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Methods for Assessing Exposure to Chemical Substances. Volume 8 Methods for Assessing Environmental Pathways of Food Contamination

Little (Arthur D.), Inc., Cambridge, MA

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Methods for Assessing Exposure to Chemical Substances

Volume 8

Methods for Assessing Environmental Pathways of Food Contamination

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16. Abstract (Limit: 200 words)

This report, one of a series of reports concerning exposure assessment, describes methods for evaluating exposure to chemical substances in food. It is intended to provide an approach for estimating human exposure to toxic substances in food when those substances enter the food through environmental pathways. This methodology provides guidelines and methods in the form of a step-by-step approach. It allows the use of available residue data, but also provides methods for identification of important contamination pathways based on chemical uses and properties. Estimation methods for some contamination pathways are suggested as well as sources of information to assist the user. An example of the application of the methodology is provided.

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METHODS FOR ASSESSING EXPOSURE TO CHEMICAL SUBSTANCES

Volume 8

Methods for Assessing Environmental Pathways of Food Contamination

by

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FOREWARD

This document is one of a series of volumes, developed for the U.S. Environmental Protection Agency (EPA), Office of Toxic Substances (OTS), that provides methods and information useful for assessing exposure to chemical substances. The methods described in these volumes have been identified by EPA-OTS as having utility in exposure assessments on existing and new chemicals in the OTS program. These methods are not necessarily the only methods used by OTS, because the state-of-the-art in exposure assessment is changing rapidly, as is the availability of methods and tools. There is no single correct approach to performing an exposure assessment, and the methods in these volumes are accordingly discussed only as options to be considered, rather than as rigid procedures.

Perhaps more important than the optional methods presented in these volumes is the general information catalogued. These documents contain a great deal of non-chemical-specific data which can be used for many types of exposure assessments. This information is presented along with the methods in individual volumes and appendices. As a set, these volumes should be thought of as a catalog of information useful in exposure assessment, and not as a "how-to" cookbook on the subject.

The definition, background, and discussion of planning exposure assessments are discussed in the introductory volume of the series (Volume 1). Each subsequent volume addresses only one general exposure setting. Consult Volume 1 for guidance on the proper use and interrelations of the various volumes and on the planning and integration of an entire assessment.

The titles of the nine basic volumes are as follows:

Volume 1	Methods for Assessing Exposure to Chemical Substances (EPA 560/5-85-001) (PB86-107083)
Volume 2	Methods for Assessing Exposure to Chemical Substances in the Ambient Environment (EPA 560/5-85-002)(PB86-107067)
Volume 3	Methods for Assessing Exposure from Disposal of Chemical Substances (EPA 560/5-85-003) (PB86-107059)
Volume 4	Methods for Enumerating and Characterizing Populations Exposed to Chemical Substances (EPA 560/5-85-004) (PB86-107042)
Volume 5	Methods for Assessing Exposure to Chemical Substances in Drinking Water (EPA 560/5-85-005) (PB86-1232156)
Volume 6	Methods for Assessing Occupational Exposure to Chemical Substances (EPA 560/5-85-006) (PB86-157211)
Volume 7	Methods for Assessing Consumer Exposure to Chemical Substances (EPA 560/5-85-007)

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1.0 INTRODUCTION

1.1 PURPOSE AND SCOPE

This document is one of a series of methodologies prepared for the U.S. Environmental Protection Agency, Office of Toxic Substances (OTS), presenting methods for estimating exposures to toxic substances from various exposure routes. This report is intended to provide an approach for estimating human exposure to toxic substances in food when those substances enter the food through environmental pathways.

The goal of this methodology is to provide a basis for examining environmental pathways of food contamination, and for estimating human exposure by those pathways. "Food" includes a variety of animal, vegetable, and mineral substances produced under a wide range of conditions. This report does not include water in its consideration of food, as that is considered in a companion volume. Potential pathways of food contamination are numerous, and methods for estimating contamination from environmental sources are almost nonexistent. This report is presented as a first attempt at an examination of the environmental pathways of food contamination. Many complex issues, such as crop uptake of chemicals, and fish bioconcentration of chemicals, are considered briefly in this report, to the extent necessary to introduce the important aspects of each issue.

This methodology presents guidelines and methods for assessing exposure to toxic substances in food, in the form of a step-by-step approach, with an explanation of the approach to and methods available for each step. Because many of the data required by each step are uncertain or unknown, the user must frequently exercise considerable judgement in completing each of the steps in the methodology.

OTS intends to use this methodology in order to assess the potential for humans to ingest certain toxic substances in their food. OTS will use such an assessment to compare the magnitude of exposures from food to the magnitudes of exposures by other routes, and determine the more important routes of exposure.

This methodology may be used by OTS to estimate food exposures to toxic substances already in commercial production (existing chemicals), or to predict potential food exposure to toxic substances before their commercialization (premanufacturing chemicals). In the case of an existing chemical, the assessment may be based on actual monitoring of environmental media, or it may be based on estimated environmental concentrations, using actual or estimated releases of the existing chemical from manufacturing, processing, industrial use, commercial use, consumer use, or accidents. For a premanufacturing chemical, the assessment may be based on monitoring data for a structure and use analogue to the premanufacturing chemical, although there are a number of problems with this approach; or it may be based on estimated environmental concentrations, using release estimates projected for the time after commercial production begins.

Depending on the scope of the assessment, OTS may use the methodology to predict food exposure from releases over a long term, e.g., manufacturing releases, or over a short term, e.g., spills. OTS may use the methodology to estimate food contamination in small geographic areas, e.g., one city, or in large geographic areas, e.g., the entire United States.

An example of a situation in which OTS has considered food contamination in some detail is a recent exposure assessment for PCBs as a result of typical spills of dielectric fluid from electrical equipment (Versar 1986). In this report, food exposure was considered in several situations, including PCBs spilled on grazing lands and farm land used to produce animal feed, on farm land used to produce vegetables, and on residential lands used to produce vegetables. The PCB assessment used some of the methods included in this methodology and many of the data sources.

It is the intent of this methodology to provide a consistent framework and a documentation of available resources for estimating food exposure.

1.2 ORGANIZATION OF THE REPORT

Section 2.0 of this report describes some approaches that have been taken by other agencies in estimating food exposure. The Food and Drug Administration (FDA), and the Office of Pesticide Programs (OPP) and the Office of Radiation Programs (ORP) in the Environmental Protection Agency all have programs which require estimates of food exposure. Generally, the approaches of FDA, OPP, and ORP are similar in that they use available data on chemical residues in food and available data on food consumption to estimate concentrations in food. ORP does attempt to estimate concentrations of radionuclides in food, but these methods are not applicable to other chemicals.

Section 3.0 describes the overall methodology, the step-by-step approach, and data sources. The basic information and methods used to estimate food exposure are described. The step-by-step approach leads the user through the process, describing the data needed, the procedures to be followed, and the results of each step. The eight steps are as follows:

1. Determine Scope of the Assessment
2. Collect Available Residue Data
3. Pathways Approach
4. Estimation of Concentration
5. Compile Concentration Data
6. Collect Consumption Data
7. Estimate Individual Dietary Intake
8. Consider Population Exposed

Section 3.0 also contains a discussion of data available on concentrations of contaminants in food, consumption patterns, and population sizes.

Section 4.0 contains a summary and examples of the use of the methodology. The step-by-step approach is applied using the chemical benzanthrone. Available monitoring data are summarized, important food contamination pathways are identified and exposures estimated for those pathways. The population exposed through the diet is also considered.

Appendix A describes the Significant Pathways Identification Methodology. This approach can be used to identify the most significant pathways for the chemical of concern by considering the production and use characteristics of the chemical, the media of release, the location and magnitude of release, and the area impacted. The physical/chemical properties of the chemical as well as the quantity of food potentially contaminated are also considered.

Appendix B describes calculational approaches for assessing the potential of pollutant migration into food. Four unique contamination pathways are identified. In the food generation stages, pathways to meat, crops, and fish/shellfish are considered. Food in the post-harvest stages is considered generally.

Appendix C describes the application of the pathways approach to the chemical benzanthrone. Quantitative methods are applied to estimate food concentrations for the most significant contamination pathways.

2.0 EXISTING METHODOLOGIES

Three government offices (U.S. Food and Drug Administration (FDA), U.S. EPA Office of Radiation Programs (ORP), and U.S. EPA Office of Pesticide Programs (OPP)) have developed approaches for evaluating exposure to chemicals in the diet. These approaches all use a combination of food consumption data (amount and type of food eaten) and information about contamination levels in those foods to estimate exposure.

The OTS methodology and the three existing approaches are most similar in their consideration of food consumption data, although the food consumption data used by FDA, OPP, and ORP are in slightly different forms. The OTS methodology draws heavily on the food consumption data used by the other offices, and it can be adapted to use food consumption data in the form used by any of these offices. The three methodologies summarized below and the OTS methodology described in Section 3 take somewhat different approaches to evaluating contaminant concentrations in foods.

2.1 U.S. EPA OFFICE OF RADIATION PROGRAMS (ORP)

ORP has developed a computer program (AIRDOS) to estimate human exposure to radioactive materials through food as a result of atmospheric releases (US EPA 1979). The doses are calculated in three phases. First, the air concentrations and deposition rates are calculated. Second, the concentrations in food items are calculated. Third, the food concentration data are used in combination with agricultural production data and food consumption data to estimate human exposure. The computer code may be used to estimate either individual exposures or annual population exposures at grid locations around the source.

Radionuclide concentrations in meat, milk, leafy vegetables, and other vegetables are calculated for two principal routes: (1) direct interception of a fraction of the deposited activity by plant surfaces, and (2) uptake of deposited activity from the soil through the plant's root system. The contamination of animal feed crop (pasture grass or stored feeds) can also be transferred to milk and meat. The concentration in vegetation is a function of the deposition flux and the fraction which is intercepted by the plant, the vegetation yield, the removal rate of the radionuclide from the vegetation, a translocation factor which relates the radionuclide concentration in the edible portion to that in the entire plant, and the time of vegetation exposure. Concentrations in plants from soil are estimated from the soil concentration and a soil-to-plant transfer factor. Concentrations in meat and milk are also calculated using transfer factors. Some statistical data are available providing these transfer factors for some radionuclides. However, such compilations have not been done for other chemicals.

The population exposed is determined by using the 1970 census enumeration district data. The consumption by the exposed population is based upon agricultural production and utilization factors large enough

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to ensure that all items produced are consumed. The user can specify the fraction of vegetables, meat, and milk that are home grown, produced in the assessment area, or imported from outside the assessment area. The average consumption values used for adults are as follows (USEPA 1979):

Food	Consumption
Leafy vegetables	18 kg/yr.
Other fresh produce	176 kg/yr.
Meat (excluding fish)	94 kg/yr.
Milk	112 liters/yr.

A more recent model to estimate risk to humans from radioactive releases has been developed at Oak Ridge National Labortory. This model (ANDROS) incorporates TERRA, a computer code that simulates terrestrial transport of radionuclides. This model functions in basically the same way as AIRDOS, however, the foods are grouped differently, and 1980 census data are used. In addition, this model can be used in conjunction with two agricultural data libraries. Agricultural production and land-use information are provided by county (AGDATC) or by ½ by ½ degree longitude-latitude grid cell (AGDATG) (Baes et al. 1985).

A similar model (POPFOOD) was developed by Nair et al. (1980) for calculating ingestion collective doses from continuous atmospheric releases of radionuclides in the United Kingdom. Their model has the same basic elements, but considers ten food products; milk; beef and veal; pork, bacon and ham; poultry meat; eggs; mutton and lamb; root vegetables; green vegetables; fruit; and cereals.

2.2 U.S. EPA OFFICE OF PESTICIDE PROGRAMS (OPP)

OPP considers dietary exposures as part of the pesticide registration process, in setting pesticide tolerances in crops and livestock, and in the process of considering the restriction of certain uses of a particular product. Their estimates of dietary exposure are based upon residue data for the food item of concern and relevant consumption data. For these purposes, OPP has developed a new Tolerance Assessment System (TAS) (USEPA 1984a). This system uses a data bank of individual food consumption patterns compiled by the U.S. Department of Agriculture to provide a system better suited to their needs. The system also contains tolerances and residue data. An exposure analysis using TAS can provide the following results on either a long term or daily basis:

- mean exposure for U.S. population and for 22 subgroups expressed as mg pesticides/kg body weight/day;
- distributions of exposure among individuals in each subgroup;
- individual commodity contributions to exposure;
- crop group contributions to exposure; and

- exposure based upon anticipated residue at the time the food is eaten[*]

Table 1 shows a summary of a TAS exposure assessment for a hypothetical chemical using a routine chronic analysis. In this analysis, a Theoretical Maximum Residue (TMRC) is calculated from the average consumption multiplied by the prior tolerances. The average consumption for each food is multiplied by a conversion factor to get a "farm gate" as opposed to an "as eaten" basis. A second calculation is done using the proposed new tolerances. Both of these are compared to some relevant dose value (RDV), which is usually an Acceptable Daily Intake (ADI). A detailed chronic analysis can be conducted, which will show a distrubtion of exposures within the subgroups. In addition, TAS can estimate acute exposure, in which food consumption estimates are for users only.

This system could be useful for assessing exposures to toxic substances if the food items in TAS are relevant to a particular exposure assessment. Access to this system can be obtained by contacting Stephen Saunders, Toxicology Branch, Hazard Evaluation Branch, OPP (703-557-2320).

As an example of OPP's approach prior to the development of TAS, Position Document 4 for ethylene dibromide (EDB) contained estimates of exposure of persons in California to this compound in fresh fruit shipped from Florida (USEPA 1983a). The mean residue level of EDB in treated oranges was 0.048 ppm. It was assumed that 1.5 kg food was consumed per day and that 1.35% of the average diet in California is fresh fruit. In addition, it was assumed that 17% of the fresh fruit consumed in California was treated. The average body weight assumed was 60 kg. Thus, the average dietary burden was estimated to be 2.75×10^{-6} mg EDB/kg body weight/day for persons in California. In addition, the USEPA (1983a) estimated exposure for "tropical fruit eaters" consuming 12 fruits/ year. This scenario was hypothetical and did not appear to be based upon consumption data. However, such assumptions can provide an upper bound on exposure. OPP also uses very localized consumption data in some cases. For the toxaphene decision document, OPP used a fish consumption survey from three counties in the Mississippi Delta area (USEPA 1982). This survey showed that 46.1% of the respondents consumed fish 1-2 times/week, and 24.5% consumed fish 2-3 times/week. The survey also showed that about 48% of the fish-eaters ate only locally caught fish, mostly from noncommercial individual fisherman. Thus, OPP's estimate of exposure to persons in this area assumed that all fish eaten were caught locally and that fish were consumed three times per week. They also assumed that each fish serving was 0.5 lbs.

These examples of OPP's approach illustrate that they use available concentration data and develop the consumption data most appropriate to

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[*] This is part of the system, but guidelines for considering pesticide dissipation or concentration due to processing are under development.

TABLE 1. SUMMARY OF EXPOSURE FOR DUMMYCIDE CALCULATED USING THE TAS ROUTINE CHRONIC ANALYSIS PROTOCOL

```
ROUTINE CHRONIC ANALYSIS: ALL STATISTICS BASED ON INDIVIDUALS' 3-DAY AVERAGE CONSUMPTION     11:43 THURSDAY, SEPTEMBER 19, 1985     1
*************************************************************************************************************************************
*************************************************************************************************************************************
*NAME: DUMMYCIDE                               STUDY    RDV        NOEL         SF     STUDY TYPE   SPECIES   EFF. LEV.   CORE GRADE   DOC. NO.*
*CASWELL NO: 900        CFR NO: CFR   .          A  00000.1000                000100 Chronic        Rat     Enzymatic   Guideline             *
*CAS NO:             SHAUGHNESSY NO:  900999     B  00000.0500                001000 Terata      Rabbit     Systemic    Minimum               *
*STATUS CODES:                                   C                                                                                         *
*RDV INFO:  The ADI value used in this analysis is  00000.1000  MG/KG  of BODY WEIGHT/DAY      (Study A)                                   *
*FILE INFO:   NEW ACTION: No User Modifications     APPROVED: Data Used        PUBLISHED:Data NOT Used                                      *
*************************************************************************************************************************************

SUMMARY BY POPULATION SUBGROUP                    TOTAL TMRC ADJUSTED FOR BODY WEIGHT        EFFECT OF NEW ACTION
==============================                    -----------------------------------        ----------------------------------------
                                                  (MG/KG BODY WEIGHT/DAY)
                                                   PRIOR TMRC    NEW TMRC     NEW TMRC        DIFFERENCE   DIFFERENCE   DIFFERENCE
                                                   (EXCLUDES    (INCLUDES    AS PERCENT       (NEW TMRC-   AS PERCENT   AS PERCENT
                                                  NEW ACTION)  NEW ACTION)      OF RDV        PRIOR TMRC)      OF RDV   OF PRIOR TMRC
                                                  -----------  -----------  ----------        ----------   ----------   ----------

U.S. POP.--48 STATES--ALL SEASONS                   0.003965     0.004757       4.757          0.000792        0.792       19.965

U.S. POPULATION--SPRING SEASON                      0.003207     0.003953       3.953          0.000746        0.746       23.263
U.S. POPULATION--SUMMER SEASON                      0.003225     0.004043       4.043          0.000819        0.819       25.384
U.S. POPULATION--FALL SEASON                        0.004759     0.005585       5.585          0.000826        0.826       17.357
U.S. POPULATION--WINTER SEASON                      0.004670     0.005446       5.446          0.000776        0.776       16.616

NORTHEAST REGION                                    0.005006     0.006014       6.014          0.001008        1.008       20.140
NORTH CENTRAL REGION                                0.003554     0.004092       4.092          0.000538        0.538       15.140
SOUTHERN REGION                                     0.003048     0.003848       3.848          0.000800        0.800       26.249
WESTERN REGION                                      0.004755     0.005611       5.611          0.000856        0.856       18.007

HISPANICS                                           0.004345     0.006386       6.386          0.002041        2.041       46.976
NON-HISPANIC WHITES                                 0.004125     0.004701       4.701          0.000575        0.575       13.946
NON-HISPANIC BLACKS                                 0.002719     0.003963       3.963          0.001244        1.244       45.755
NON HISPANICS OTHER THAN BLACKS & WHITES            0.004239     0.008156       8.156          0.003917        3.917       92.405

NURSING INFANTS (<1 YEAR OLD)                       0.029904     0.032966      32.966          0.003062        3.062       10.238
NON-NURSING INFANTS (<1 YEAR OLD)                   0.040317     0.046927      46.927          0.006610        6.610       16.396
FEMALES(13+,PREGNANT, NOT NURSING)                  0.002433     0.002999       2.999          0.000566        0.566       23.264
FEMALES(13+,NURSING)                                0.003091     0.003739       3.739          0.000649        0.649       20.985
CHILDREN(1-6 YRS)                                   0.013638     0.015234      15.234          0.001596        1.596       11.702
CHILDREN(7-12 YRS)                                  0.005324     0.006340       6.340          0.001016        1.016       19.087
MALES(13-19 YRS)                                    0.002464     0.003119       3.119          0.000655        0.655       26.595
FEMALES(13-19 YRS,NOT PREG. OR NURSING)             0.002488     0.003068       3.068          0.000580        0.580       23.299
MALES(20+ YRS)                                      0.001776     0.002475       2.475          0.000699        0.699       39.356
FEMALGS(20+ YRS,NOT PREG. OR NURSING)               0.001975     0.002438       2.438          0.000463        0.463       23.456

ALASKA                                              0.000000     0.000000       0.000              .            .            .
HAWAII                                              0.000000     0.000000       0.000              .            .            .
PUERTO RICO                                         0.000000     0.000000       0.000              .            .            .
LOW INCOME- 48 STATES                               0.000000     0.000000       0.000              .            .            .
```

Source: Saunders and Petersen 1986

the situation. In many cases, the consumption data have been gathered for a particular food item in a particular area of the country.

2.3 U.S. Food and Drug Administration (FDA)

The FDA has several approaches which estimate or actually measure human exposure through food. The agency conducts yearly Total Diet Studies. These studies represent a monitoring program intended to provide an estimate of the actual dietary intake of pesticides, PCBs, toxic elements, radionuclides, essential minerals, and other contaminant residues. Market baskets representative of foods consumed are collected from various parts of the country, prepared as for consumption, and analyzed. Intakes are estimated for various age groups based upon consumption patterns in the USDA's Nationwide Food Consumption Survey (NFCS) and the Health and Nutrition Examination Survey (NHANES II). The total diet study now includes representative diets for eight age and sex groups, including infants, toddlers, teenage males, teenage females, adult males and females and older males and females. Foods are purchased in four geographic regions of the country. The diets consist of 234 foods which represent 90% or more (by weight) of the foods generally consumed by persons in the U.S. The consumption patterns are based on the NCFS and the NHANES food consumption studies (see Section 3.2.2). The agency also carries out extensive monitoring of domestic and imported foods for these residues with emphasis on the raw agricultural commodity.

The Division of Food and Color Additives of FDA reviews petitions for marketing of new compounds, including food additives, color additives, and animal drugs. They also conduct retrospective reviews of approved compounds. In the review of additives, they assess human exposure by considering the proposed use and consumption data for the food of interest (USFDA 1982).

FDA developed a food consumption model to estimate dietary intake of lead, an inadvertent contaminant in food (Beloian 1981). This model used three variables. The number of eating occasions and mean serving size were used along with mean lead content of foods. This approach is slightly different than most other approaches, which use USDA food consumption data.

2.4 SUMMARY

In the broad sense, the approaches of FDA, OPP, and ORP are basically the same in that they use available data (or estimates based on available data) of levels of chemical residues in food, and available data on food consumption to estimate exposures from food. ORP also attempts to estimate concentrations of radionuclides in food where residue data are not available, but ORP's methods are not immediately useful for other chemicals, for which chemical-specific transfer factors are unavailable.

The approach presented in this methodology draws from the existing FDA, OPP, and ORP approaches where possible. None of these approaches is completely applicable to the types of exposure estimates envisioned in this methodology. Where residue data are not available, the approach in this methodology is to attempt to predict concentrations of residues, unlike the approaches of FDA and OPP. Although ORP also attempts to predict residue concentrations where necessary, the methods for radionuclides are not easily used for other chemicals. This methodology presents ORP's estimation techniques, but it also presents a number of other techniques more useful for the chemicals of interest to OTS.

Although, as mentioned above, the approach in this methodology can use food consumption data in the form it is used by FDA, OPP, or ORP, it can also be adapted to use other types of food consumption data, such as data from surveys made in a limited geographic area on one food item.

3.0 OVERALL METHODOLOGICAL FRAMEWORK

3.1 APPROACH

3.1.1 General discussion

The basic framework for estimating exposure to a pollutant in the diet is shown in Figure 1. This very simple diagram illustrates that estimating dietary intake (E in mg/day) requires information on the concentration (C_f in mg/kg) of the pollutant in the food or food group at the time of consumption and on the amount of the contaminated food consumed (L in kg/day). The concentration of the pollutant in various food items may represent measured values or estimated concentrations. The consumption of the food item may be an average value for the U.S. population or region-specific, or may be a distribution of values for individuals. This section will describe how measured concentrations can be used to estimate food exposures, as well as how a pathway approach can be used to identify potential mechanisms of food contamiation. Estimates of food concentrations can then be developed specifically for these pathways.

While using measured values for L and C_f in Figure 1 can be simple, trying to estimate values for E is complex, because each food and food group has different characteristics and processing methods associated with it. Thus,

$$E_T = \sum_{i=1}^{n} (C_f)_i (L)_i \qquad (3\text{-}1)$$

for all the different foods or food groups to be considered, where E_T equals total dietary exposure. The food groups used in food consumption studies provide a good basis for estimating exposure (USDA 1980). Table 2 shows the food groups used as a framework for estimating exposure. Also shown in this table are the consumption, percent fat, and the major food items of the group. This table points out foods of particular interest because of high consumption rates or high fat content. The latter foods might be important to consider due to the tendency of some pollutants to bioconcentrate in fats. For a particular assessment of food exposure, it may be necessary to consider specific food items. For example, it may be of interest to separate leafy vegetables from root crops. The food groups in Table 2 are provided as a basis for a general consideration of food exposure.

Figure 2 shows how dietary intake would be estimated from the intakes calculated for various foods or food groups. The primary food within a food group, as identified in Table 2, is shown in the boxes in Figure 2.

It may be necessary to consider different processing methods within a food group, especially for fruits and vegetables. As an example, Figure 3 shows how E_V, the dietary intake from vegetables, would be estimated; the estimation of E_F, the dietary intake from fruit, would be similar. Table 3 shows the per capita consumption of

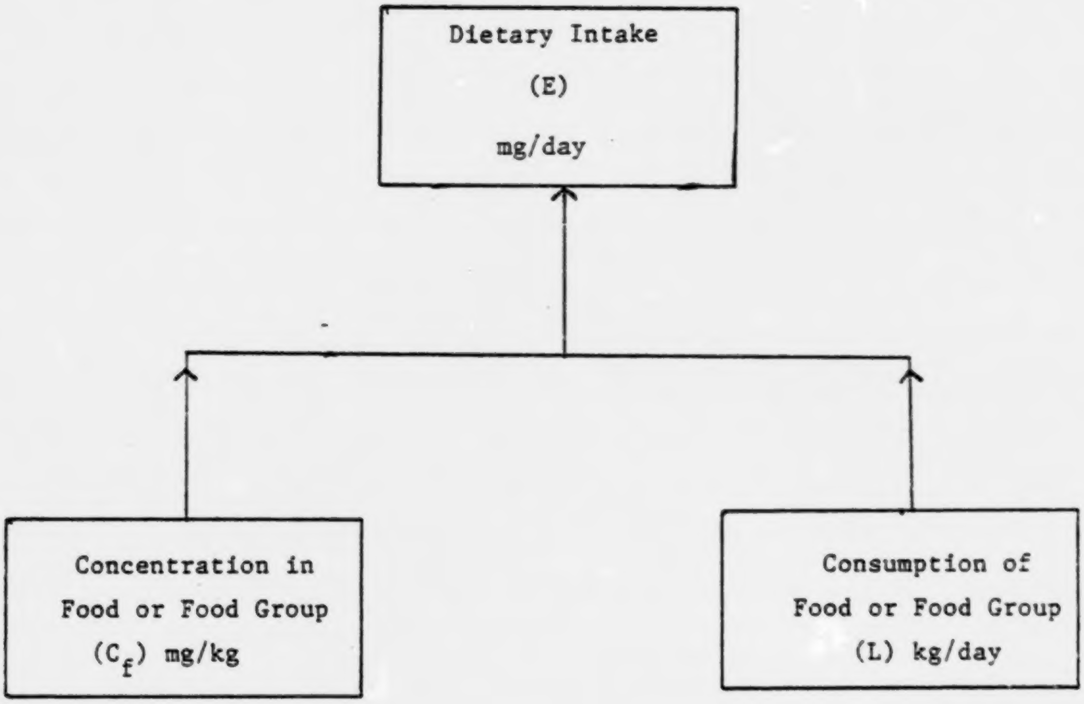
Dietary Intake
(E)
mg/day
Concentration in
Food or Food Group
(C_f) mg/kg
Consumption of
Food or Food Group
(L) kg/day

FIGURE 1. SIMPLE FRAMEWORK FOR ESTIMATING DIETARY INTAKE

TABLE 2 ' FOOD GROUPS

Food Group	Consumption* gram/day	% Fat	Major Food Item (consumption grams/day)
Meat	169	5-45	beef (54)
Poultry	27	5-20	chicken (24)
Fish/Shellfish	11	0.3-3	---
Milk & Milk Products	352	0.1-4	milk (242)
Eggs	27	11.5	eggs
Fats & Oils	14	100	shortening
Legumes, nuts, seeds	26	40-65	
Grain Products	204	1-2	wheat or whole wheat flour
Sugar & Sweeteners	23+	0	cane and beet sugar
Vegetables	201	0.1-0.7	potatoes (64)
Fruit	142	0.2-0.6	citrus fruit juices (57)
Beverages	667	0	coffee (262)

Source: USDA (1980, 1981).

* Average consumption per individual including all age groups (USDA 1980)

+ Does not include sugar or sweeteners which are ingredients in other foods.

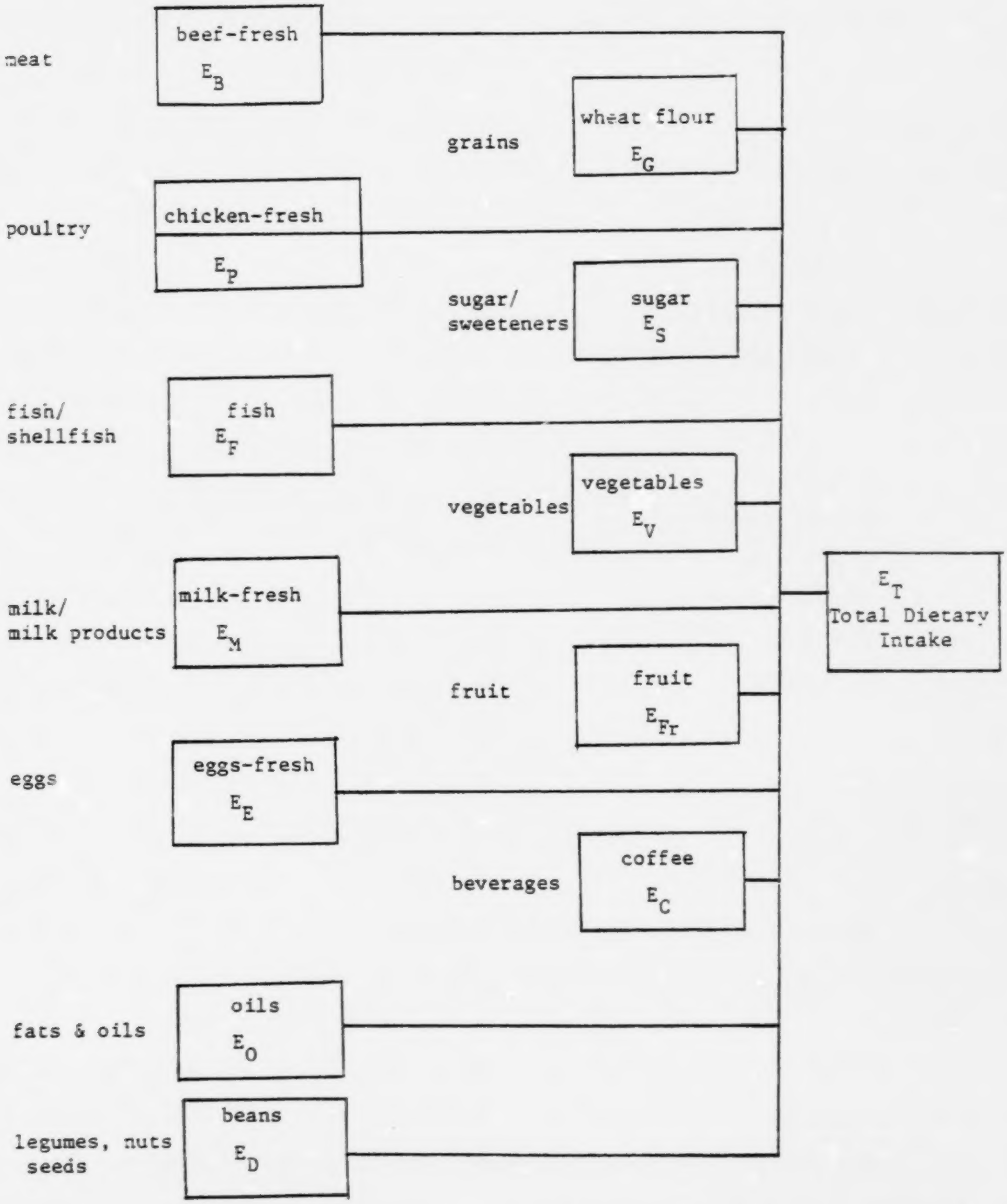
meat
beef-fresh
E_B
grains
wheat flour
E_G
poultry
chicken-fresh
E_P
sugar/
sweeteners
sugar
E_S
fish/
shellfish
fish
E_F
vegetables
vegetables
E_V
E_T
Total Dietary
Intake
milk/
milk products
milk-fresh
E_M
fruit
fruit
E_{Fr}
eggs
eggs-fresh
E_E
beverages
coffee
E_C
fats & oils
oils
E_O
legumes, nuts
seeds
beans
E_D

FIGURE 2. FRAMEWORK FOR ESTIMATING DIETARY EXPOSURE FROM FOODS OR FOOD GROUPS

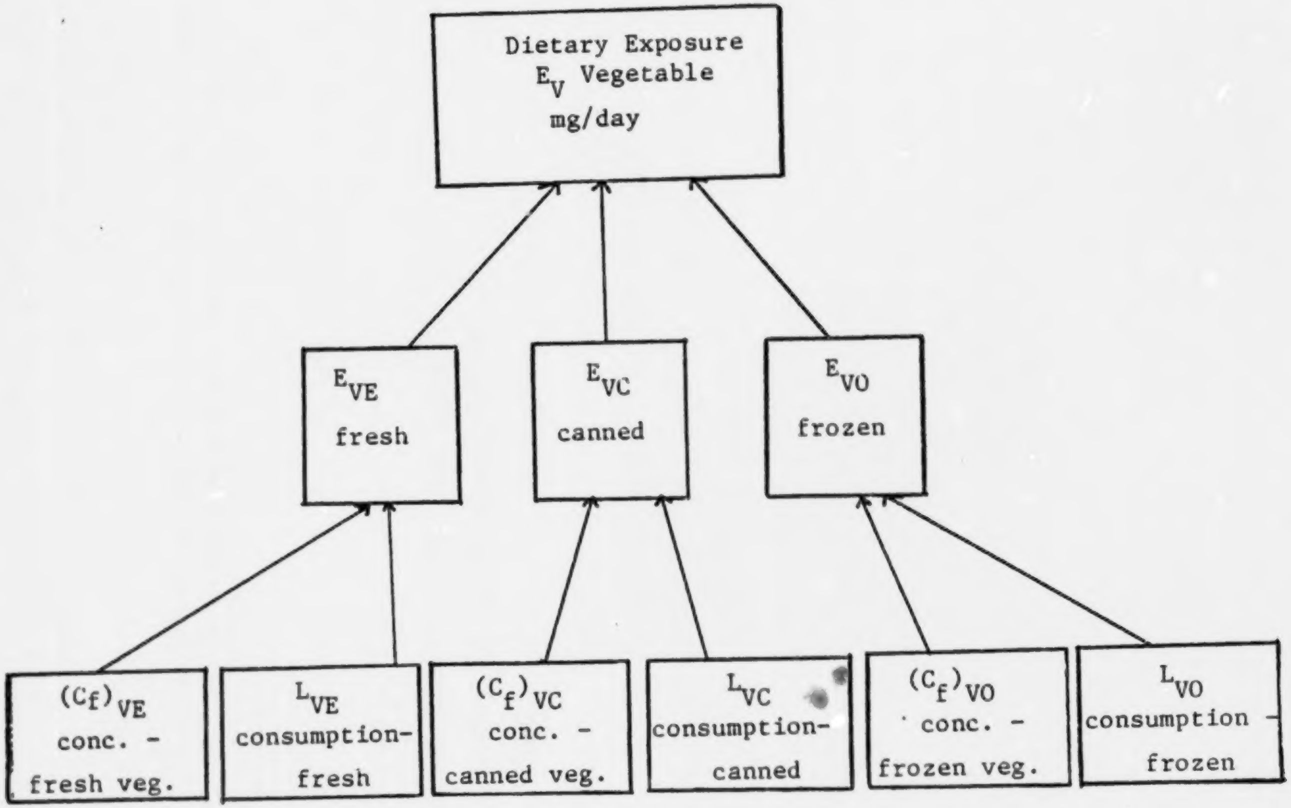
Dietary Exposure
E_V Vegetable
mg/day
E_{VE}
fresh
E_{VC}
canned
E_{VO}
frozen
$(C_f)_{VE}$
conc. -
fresh veg.
L_{VE}
consumption-
fresh
$(C_f)_{VC}$
conc. -
canned veg.
L_{VC}
consumption-
canned
$(C_f)_{VO}$
conc. -
frozen veg.
L_{VO}
consumption -
frozen

FIGURE 3. ESTIMATION OF DIETARY EXPOSURE FROM VEGETABLES

TABLE 3 CONSUMPTION OF FRUITS AND VEGETABLES (1980)*

Product	Per Capita Consumption (grams/day)
Vegetables	260.6
fresh	185.9
canned	61.8
frozen	12.9
Fruits	174.1
fresh	104.2
processed (mostly frozen citrus juices and canned fruits and juices)	69.9 (fresh equivalent)

---

*Note: These consumption values are slightly different from those shown in Table 3-1 due to differences in food group definition used in the two documents.

Source: USDA (1981).

fruits and vegetables by process category. Thus, various combinations of these intakes might be utilized, although in general it would be important to consider the food/process category with the highest consumption.

The above discussion may imply that in order to estimate dietary intake, one must have concentration data for all the food groups shown in Table 2 and Figure 2. While this may be the ideal, such data are rarely available. In order to provide a focus to an assessment, a pathway approach can be used. The goal of this approach is to identify the most important pathways of contamination for food. These pathways may be specific to type of food, process, or area of the country, depending on the nature of the uses and releases of the compound. Once the most significant pathways are identified, monitoring data can be evaluated for its relevance and completeness and estimation techniques can be focused on these pathways, thus limiting the scope of the assessment as desired.

Figure 4 shows the potential contamination pathways of a pollutant to food. This diagram is for illustrative purposes only, as the complexity of this diagram reinforces the need to prioritize the pathways in some way. There are several factors which influence the significance of contamination pathways:

- the nature of the chemical use
- the chemical and physical properties of the pollutant
- the nature of the food

The nature of the chemical's uses will affect where it is released and potential points of contact with food, as shown in Figure 4. The physical and chemical properties of the compound will affect its persistence in any media contacting food, and its propensity to be associated with particular food items. The nature of the food would affect its ability to take up, absorb, or otherwise accumulate the compound of concern.

The significance of various contamination pathways needs to be evaluated on several different levels. On the simplest level, the magnitude of the resultant concentration in food is the criterion, with a higher concentration reflecting a more significant contamination pathway. On another level, consumption patterns must be considered to judge the significance, based on actual human exposure (see Figure 1). In addition, however, the proportion of the total food supply (or the size of the subpopulation) potentially affected is an important criterion in establishing the significance of a given pathway. All of these criteria must be accommodated at some point in a methodology to identify significant pathways of food contamination.

It should be pointed out that the pathways described above and shown in Figure 4 imply that a chemical will be used in a certain way. However, the potential for an accident or misuse always exists. In fact, many of the significant food contamination incidents are a result of unexpected pathways. This methodology addresses some possible

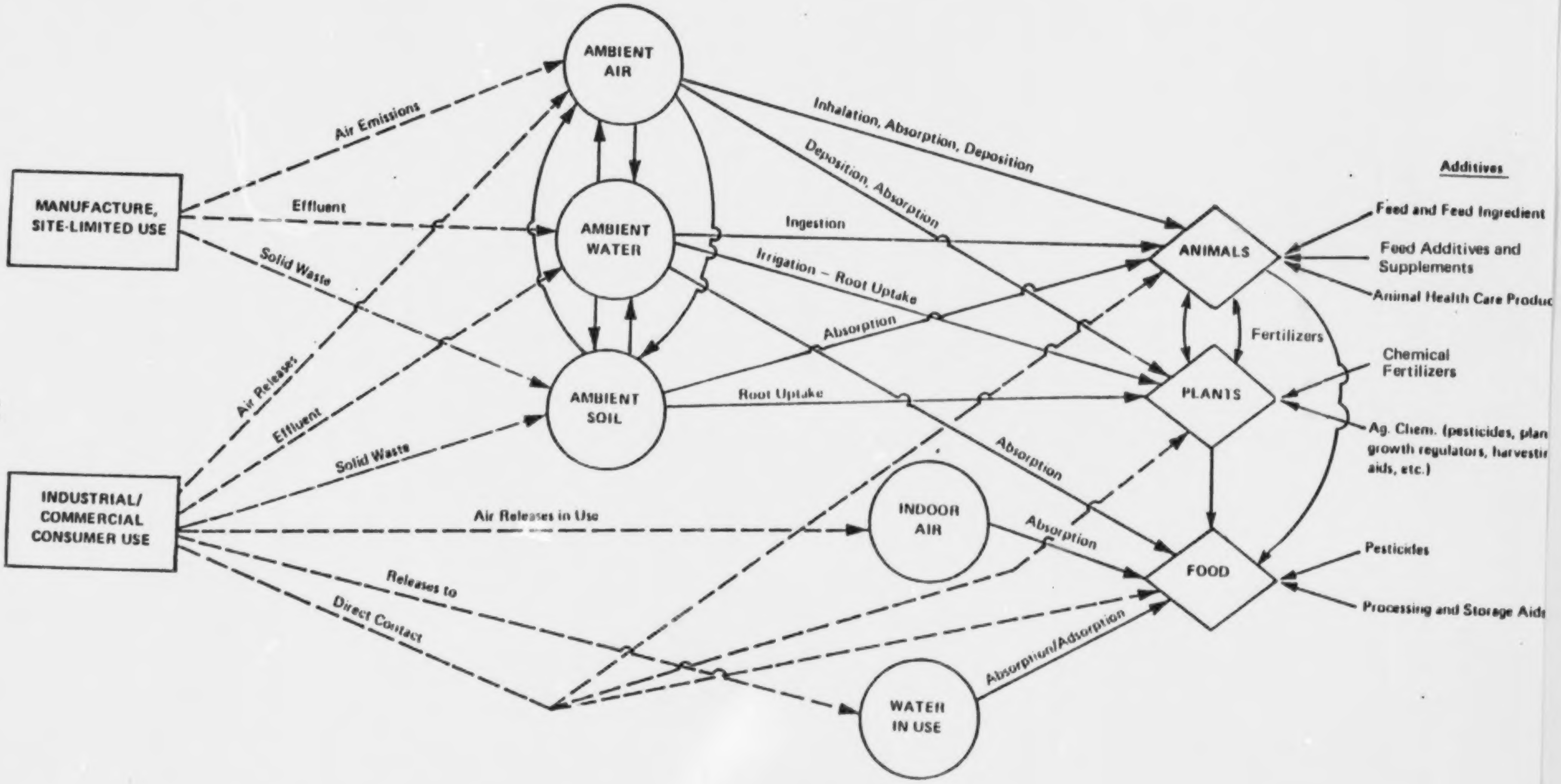
MANUFACTURE,
SITE-LIMITED USE
INDUSTRIAL/
COMMERCIAL
CONSUMER USE
Air Emissions
Effluent
Solid Waste
Air Releases
Effluent
Solid Waste
Air Releases in Use
Releases to
Direct Contact
AMBIENT AIR
AMBIENT WATER
AMBIENT SOIL
INDOOR AIR
WATER IN USE
Inhalation, Absorption, Deposition
Deposition, Absorption
Ingestion
Irrigation – Root Uptake
Absorption
Root Uptake
Absorption
Absorption
Absorption/Adsorption
ANIMALS
PLANTS
FOOD
Fertilizers
Additives
Feed and Feed Ingredient
Feed Additives and Supplements
Animal Health Care Produc
Chemical Fertilizers
Ag. Chem. (pesticides, plan growth regulators, harvestir aids, etc.)
Pesticides
Processing and Storage Aid

FIGURE 4 PATHWAYS OF FOOD CONTAMINATION

routes of accidental contamination, but does not provide specific methods for estimating exposure resulting from such contamination.

3.1.2 Step-by-Step Approach

This section provides a step-by-step approach for assessing human exposure to chemical contaminants in food. It makes use of any available monitoring data as well as a pathways approach to identify food items that might be contaminated. Quantitative methods are presented to provide what is generally a rough estimate of concentrations in food.

The step-by-step approach is summarized in Table 4 and discussed by step in the following Sections.

3.1.2.1 Step 1 Determine the Scope of the Assessment

The scope of the assessment is a function of the objectives of the study, which may range widely. It may be important to provide a very rough estimate of food exposure for comparison with other exposure routes. In contrast, a very detailed analysis of food exposure may be required in some situations. The scope also needs to be consistent with the data available. For example, in the evaluation of a new chemical, no monitoring data are available for food. In addition, limited information is available on the chemical's potential uses and releases. Therefore, the scope and objective of such an analysis must be realistic. For an existing chemical, a considerable amount of data may be available, and the scope is limited by other constraints.

The determination of the objectives also involves a consideration of the desired type of representation of exposure. Both residue data and food consumption data may be utilized as an average or mean, a distribution, or a maximum. While it is desirable to use a consistent approach throughout the analysis, this is not always possible. For example, in many cases mean residue data are used in combination with a distribution of consumption patterns or a mean and worst case. Such an approach was used by EPA in their consideration of exposure to EDB in citrus, as described in Section 2.2.

The population exposed can also be considered on different levels. In some cases, a site-specific assessment may be required, while a national assessment is required in other cases.

The result of Step 1 should be a well-defined scope for the assessment of food exposure, as shown in Table 4. Of course, as the assessment progresses, modification to the scope may be needed, based upon unforeseen data gaps or other unexpected problems.

3.1.2.2 Step 2 Collect Available Residue Data for Food

This section involves a search of the literature, if it is an existing chemical, for data on residues of the chemical in items of the U.S. diet. The extent to which the literature is searched and food items are included may be limited by Step 1, the scope of the

TABLE 4. Step-by-Step Approach

Step	Inputs or Data Required	Results	Specific Method or Sources of Information
1. Determine Scope of the Assessment	● Time Frame ● Budget ● Goals of the Assessment ● New or Existing Chemical	Specific Scope of the Assessment - average, worst case, or distribution of exposure - limits on data acquisition - national or site-specific	This section
2. Collect Available Residue Data	● Specific chemical or form of interest ● Specific foods of interest, if specified	● A collection of sampling and analysis data for chemicals by food items of the diet	Section 3.2.1
3. Pathways Approach	● Chemical uses ● Fate analysis ● Chemical properties ● Agricultural statistics	● An identification of most significiant contamination pathways	Appendix A
4. Estimation of Concentration	● Chemical Properties ● Food characteristics ● Environmental concentration	● Estimated concentration in food	Appendix B
5. Compile Concentration Data	● Output from Steps 1,2,4	● Compilation of concentration data by food or food group in the desired format	This section
6. Collect Consumption Data	● Food or Food groups of interest ● Output from Step 1	● Compilation of consumption level by food or food group in the desired format	Section 3.2.2

TABLE 4. Step by Step Approach

Step	Inputs or Data Required	Results	Specific Method or Sources of Information
7. Estimate Individual Dietary Intake	● Output from Steps 5 and 6	● Estimate of dietary intake by food or food group and total dietary intake	This section
8. Consider Population Exposed	● Output from Step 7	● Size of population associated with various dietary intakes	Section 3.2.3

assessment. The sources of information for concentrations of pollutants in food can be found in Section 3.2.1. For a new chemical, it may be possible to use available data on a structure and use analogue. At this point, it may be important to consider possible metabolites or degradation products of the chemical. Additional data may be available for levels of these compounds in food.

The results of Step 2 will provide a compilation of residue data in food by food type or group. If no data are available, the user should proceed to Step 3. When data are available, Step 3 can be used to confirm or supplement it. If this is not desirable, the user should go to Step 5.

3.1.2.3 Step 3 Pathways Approach

If monitoring data collected in Step 2 are inadequate and if the scope of the assessment and the time available allow, the pathways approach can be used to identify the most significant pathways of contamination for food. This approach is described in Appendix A in detail and will result in an assessment of the type of food, and the areas of the country which are most likely to be contaminated based upon the chemical's use and release characteristics and its physical and chemical properties.

The results of Step 3 can be used in one of two ways. First, the results can be used to evaluate the residue data in order to determine whether the available data are representative of the contamination pathways predicted to be the most significant. If not, then the second approach could be used to estimate concentrations by these pathways using quantitative methods in Step 4.

3.1.2.4 Step 4 Estimate Concentrations in Food - As Eaten

Step 1 and Step 3 will determine the extent to which quantitative methods should be applied. The methods available are described in Appendix B in four major categories. In the food generation stages, pathways to meat, crops, and fish/shellfish are considered. In the post-harvest stages, food is considered as a whole, as contamination pathways are more dependent on processing method than on food types. It is important in this process to consider the food from the point of contamination to the consumer. For example, if wheat in the growing stages is thought to be contaminated, then various products need to be evaluated such as wheat flour or ready-to-eat baked goods. In addition, while it is recognized that metabolism or degradation of chemicals may result in more toxic compounds, such considerations are far too complex for the general methodology at this time. If data exists on a specific chemical being considered, these data should be incorporated into the assessment.

Of the methods that are provided in Appendix B, some have been empirically developed, while others are presented based upon similar processes in other media. Most have not been validated for the purposes which they are intended in this methodology, and none have been developed using a data base including a large set of chemicals.

These qualifications are presented as a caution for the use of these models and the precision which can be attached to the results. With these qualifications in mind, however, the results of Step 4 can be used to provide concentration data for exposure estimates.

3.1.2.5 Step 5 Compile Food Concentration Data

In Step 5, the concentration data from Steps 2 and 4 will be compiled. It should be organized by food group (See Table 2), with data on specific foods together. At this point, it would be useful to present the concentration data as they will be used in the exposure assessment. This presentation has been determined in Step 1, i.e., mean, maximum, or distributions of data. The results from this step can then be used directly to estimate exposure.

3.1.2.6 Step 6 Collect Appropriate Consumption Data

In the previous steps, the foods or food groups of interest have been determined. In order to estimate exposure, the levels of consumption are needed for these foods. The types of data available on consumption patterns are described in Section 3.2.2. The particular data chosen will depend upon the scope of the assessment as determined in Step 1. It may be desirable to use an average consumption for the U.S. or an average consumption for those persons consuming the product (users). In a more detailed analysis, a distribution of consumption patterns may be used. In some situations, the use of a maximum consumption value may be the most appropriate. Consumption patterns that are very limited, either geographically or by food, may be desirable and available in some cases. In other cases, assumptions must be made based upon available information.

The result of Step 6 is a set of consumption levels corresponding to the concentration data for food items developed in Step 5 and in the desired format as specified in Step 1.

3.1.2.7 Step 7 Estimate Individual Dietary Intake

The estimation of individual dietary intake using Equation 3-1 is straightforward once Steps 5 and 6 have been completed. Of course, these estimates represent intakes as defined by the concentration data and consumption data. For example, if concentrations vary geographically or with distance from a source, exposures would be estimated to correspond to the various concentration levels. Step 1 will define these considerations to some extent. In addition, the variation in food concentrations as determined by the monitoring data or the fate analysis will affect the ability or need to differentiate exposure groups.

The result of Step 7 will be a quantification to the extent possible of the dietary intake of the chemical of interest. The intake should be presented as defined in Step 1. It may be presented by food or food group and may be specific to exposure groups or populations.

3.1.2.8 Step 8 Consider Population Exposed

Step 7 estimates the individual exposure for a variety of exposure groups or populations. Step 8 involves the evaluation of the numbers of persons in each of these groups. The amount of food potentially contaminated, as estimated in Step 3, will determine the minimum potential population size exposed (although the maximum exposure). The example of OPP's exposure assessment described above in Section 2.2 showed that they had specific information on the distribution of citrus fruits shipped from Florida to California. In general, however, such information is not easily obtainable. Two different options for quantifying the population exposed can be used, depending upon the consumption pattern information utilized. These options are as follows:

$$P_f = \frac{T_f}{L_f\ 365} \qquad (3\text{-}2)$$

Where P_f = the number of persons exposed to the pollutant from consuming a particular food, T_f = the total amount of the food potentially contaminated in kg/year, and L_f = the consumption pattern for that food in kg/day. This method obviously assumes that all food produced is consumed and that 100% of the person's diet of the particular food item is contaminated. Alternatively, all users of the food item in the U.S. could be exposed, with the contaminated product representing a portion of their consumption of that food item:

$$F = \frac{T_f}{R} \qquad (3\text{-}3)$$

where F = the fraction of the food item produced yearly that is contaminated, and R = the total amount of the food produced per year (kg). On the average, the actual consumption of the contaminated product (A_f in kg/day) can be estimated by:

$$A_f = F\ L_f \qquad (3\text{-}4)$$

These two options represent a wide range for the exposed population. The first alternative is more appropriate when production and consumption are confined to a local area. The second alternative should be used when the contaminated product is known to be widely distributed.

The population exposed would be determined by food or food group and would be consistent with assumptions made about consumption patterns.

3.2 DATA SOURCES

There are many pieces of data that are needed in the application of the methodology for estimating the dietary intake of a chemical. The two parts of the equation are the concentration in the food and the consumption of the food as shown in Figure 1. In general, three types of data are needed, each at various points in the general methodology described. They are: concentration data, consumption data, and population data. Data sources and data bases for each of these categories are described below.

3.2.1 Concentration Data

Information on concentrations of pollutants in foods or food groups is very scattered in the literature. There is no data base containing a compilation of the existing data on residues. The following list gives some potential sources of concentration data:

- Pesticides Monitoring Journal, Journal of the Association of Official Analytical Chemists

  Results of FDA's Total Diet Studies, primarily for pesticides and industrial chemicals such as PCB's and toxic elements. Results of FDA's monitoring of domestic and imported food, primarily for pesticides, industrial chemicals and toxic elements.

- STORET

  U.S. EPA Monitoring and Data Support Division, Office of Water - Water Quality Data Base - contains fish tissue data from a variety of sources for a number of pollutants.

- USDA

  Food Safety and Inspection Service - collects nationwide samples of meat and poultry at slaughter establishments, analyzed for animal drugs, pesitides, and other chemicals. Date can be retrieved by zip code of the seller or packing plant.

- U.S. EPA - Office of Pesticide Programs

  Residue Chemistry Branch - residue data for registered pesticides in raw agricultural commodities.

- States

  Some states have monitoring programs particularly for pesticides and a few other chemicals; monitoring data for fish may also be available.

In searching for data for a particular contaminant in food, a literature search would be required, covering both agricultural and environmental journals. Several journals publish data on measurements of pollutant concentrations in fish, animals, and crops. Among these are journals such as Residue Reviews, Journal of Agriculture and Food Chemistry, Environmental Science and Technology, Bulletin of Environmental Contamination and Toxicology, Journal of Food Technology, and Journal of Food Science. However, many of the surveys are very region-specific and may be found in journals published and distributed in that region. A comprehensive literature search would be required to ensure the collection of all food monitoring data. In some assessments, regulatory levels can be used instead of actual monitoring data. Tolerances that are established for toxic substances in or on raw agricultural commodities or in processed foods could be used in an exposure assessment. These levels are used in exposure assessments by OPP as shown in Table 2. The GRAS allowable levels could be used in a similar manner. The use of such indices would provide a worst case assessment, as they represent maximum allowable levels.

3.2.2 Consumption Data

Depending on the contamination pathway under consideration, different types of data on food consumption patterns will be required as input into the equation to estimate dietary intake. The primary data source for food consumption patterns is the 1977-78 household survey of food consumption conducted by the U.S. Department of Agriculture, the Nationwide Food Consumption Survey - NFCS (USDA 1980). A sample of 15,000 households and 34,000 individuals was included in the basic survey of the 48 conterminous states for each of four quarters from April 1977 through March 1978. Supplemental surveys were conducted to include: elderly persons; households eligible for the Food Stamp Program; urban households; and households in Alaska, Hawaii and Puerto Rico. In all cases, except the supplemental survey of elderly persons, dietary intake was recorded for three consecutive days. The food data base contains 3727 foods. This report (USDA 1980) provides average consumption levels for individuals (by age) or households, region of the country, income, season of the year, and level of urbanization. Food items are covered quite specifically, and food sources (i.e., bought, home produced) are considered to some degree. Food processing methods are also differentiated, including data on fresh, frozen, dried, and canned foods. Table 2 summarizes results for all individuals for major food groups and Table 5 shows an example of data on consumption of meat, poultry, and fish for all age categories. While these data should be adequate for most purposes, there are some deficiencies. For example, USDA (1980) presents average daily consumption patterns. The data base, however, contains all the individual consumption patterns, so distributions are possible as the data base has been computerized by USDA.

Pao et al. (1982) has published a report based upon the USDA Nationwide Food Consumption Survey. Their report summarizes the percent of individuals using particular food items in the three days for which dietary information was available (users) and the average consumption per day by users at specified percentiles. The maximum in any one day, as well as the maximum over three days is also reported. Consumption patterns are differentiated by age and sex of individual, but not by area of the country. Specific foods which were most commonly reported by individuals are included in this report. Table 6 shows an example of these data for beef steaks.

In general, these two data compilations are adequate for most exposure assessments. The NFCS data provide average intakes by various groups for a wide variety of foods. The data from this survey summarized by Pao provides additional information an average and distribution of intakes for users, as well as a maximum intake for one day. These data would be useful for worst-case assessments or where acute affects are of concern.

TABLE 5

MEAT, POULTRY, FISH
Average intake[1] per individual in a day,[2] spring 1977
48 States, all urbanizations, all incomes

Sex and age (years)	Individuals	Meat, poultry, fish: Total	Beef	Pork	Lamb, veal, game	Poultry: Total	Poultry: Chicken	Organ meats, mixtures mainly organ meats	Frankfurters, sausages, luncheon meats, spreads	Fish, shell-fish	Mixtures mainly meat, poultry, fish
	Number	Grams									
Males and females:											
Under 1	[3]78	72	9	4	3	4	1	0	2	0	51
1-2............	[4]264	91	18	6	([5])	16	13	([5])	15	4	32
3-5............	437	121	23	8	([5])	19	19	1	15	6	49
6-8............	469	149	33	15	1	20	19	1	17	7	55
Males:											
9-11...........	216	188	41	22	3	24	21	1	19	7	71
12-14...........	313	218	53	18	([5])	27	24	([5])	25	8	87
15-18...........	400	272	62	24	1	37	32	3	25	7	93
19-22...........	287	310	90	21	2	45	43	1	33	6	112
23-34...........	770	285	86	27	1	31	29	2	30	14	94
35-50...........	784	295	75	28	1	31	28	3	26	17	113
51-64...........	634	274	70	32	1	31	29	4	29	22	86
65-74...........	295	231	54	25	2	29	26	5	22	21	72
75 and over.....	127	196	41	39	7	28	25	4	19	5	54
Females:											
9-11...........	241	162	38	17	1	27	23	0	20	5	55
12-14...........	309	176	47	19	1	23	22	1	18	7	61
15-18...........	402	180	46	14	2	28	27	1	16	11	61
19-22...........	337	184	52	19	1	26	24	([5])	18	8	61
23-34...........	949	183	48	17	1	24	22	1	16	10	66
35-50...........	942	187	49	19	2	24	21	2	14	14	63
51-64...........	792	187	52	19	2	26	24	4	12	12	60
65-74...........	377	159	34	21	4	30	25	2	12	9	47
75 and over.....	197	134	31	17	2	19	16	3	9	4	49
All individuals...	[6]9,620	207	54	20	2	27	24	2	20	11	72

---

[1] Quantities given are for foods as ingested; no inedible parts are included.

[2] Based on 24-hour dietary recall of day preceding interview.

[3] Excludes 36 breast-fed infants.

[4] Excludes 4 breast-fed infants.

[5] Less than 0.5 g but more than 0.

[6] Excludes 40 breast-fed infants.

Source: USDA 1980

TABLE 6 Beef Steaks Consumed in 3 days by Individuals, As States, 1977 - 1978

MEASURE AND UNIT	TOTAL	AGE (YEARS) AND SEX OF INDIVIDUAL				AGE (YEARS) AND SEX OF INDIVIDUAL--CONTINUED											
		UNDER 1	1-2	3-5	6-8	9-14		15-18		19-34		35-64		65-74		75 AND OVER	
		MALE AND FEMALE	MALE AND FEMALE	MALE AND FEMALE	MALE AND FEMALE	MALE	FEMALE	MALE	FEMALE	MALE	FEMALE	MALE	FEMALE	MALE	FEMALE	MALE	FEMALE
TOTAL INDIVIDUALS 1/ (WEIGHTED).............NUMBER....	37,874	498	1,045	1,719	1,841	2,089	2,158	1,394	1,473	3,928	5,346	4,929	7,069	1,118	1,738	536	993
TOTAL INDIVIDUALS USING FOOD:																	
AT LEAST ONCE IN 3 DAYS.....................PCT......	27.6	2.3	19.5	24.2	25.6	24.5	25.9	27.3	23.7	31.8	27.1	35.0	30.3	25.0	23.3	24.8	18.1
ON ONLY 1 OF 3 DAYS.......................PCT......	23.4	2.1	16.8	21.6	23.6	21.8	23.0	24.0	21.0	26.2	23.4	27.4	25.2	20.6	19.8	21.9	14.9
ON ONLY 2 OF 3 DAYS.......................PCT......	3.9	.1	2.3	2.4	1.8	2.6	2.6	3.1	2.6	5.0	3.3	6.6	4.8	3.9	3.3	2.0	3.0
ON ALL 3 OF 3 DAYS........................PCT......	.4	.1	.4	.2	.1	0	.2	.2	.1	.6	.4	1.0	.3	.5	.1	.8	.1
EATING OCCASIONS AT WHICH ITEM WAS CONSUMED IN 3 DAYS BY USERS:																	
AVERAGE 1/ ....NUMBER....	1.2	1.2	1.2	1.1	1.1	1.1	1.1	1.2	1.1	1.2	1.2	1.3	1.2	1.3	1.2	1.3	1.2
STANDARD DEVIATION..........................DO......	.5	.5	.5	.4	.3	.3	.4	.4	.4	.5	.4	.6	.5	.6	.5	.6	.5
MAXIMUM.....................................DO......	6.0	3.0	3.0	4.0	3.0	3.0	3.0	3.0	3.0	6.0	4.0	6.0	5.0	5.0	4.0	4.0	3.0
QUANTITY CONSUMED BY USERS:																	
USED AT LEAST ONCE IN 3 DAYS:																	
AVERAGE PER DAY 1/ ....GM......	65	17	24	29	39	51	47	6'	56	90	63	84	69	67	53	71	56
STANDARD DEVIATION........................GM......	51	10	16	24	29	34	31	51	40	74	41	56	45	40	34	43	41
AVERAGE PER DAY AT SPECIFIED PERCENTILES: 1/																	
5TH.......................................GM......	15		5	8	12	15	14	19	18	24	19	28	19	23	18	23	14
25TH......................................GM......	31		12	15	23	31	28	37	31	54	37	47	37	37	31	37	28
50TH......................................GM......	56		19	27	31	38	37	60	46	75	56	75	56	56	46	61	46
75TH......................................GM......	75		31	37	46	61	56	84	65	112	75	112	75	77	67	82	75
90TH......................................GM......	123		46	51	68	85	75	117	107	160	120	149	123	122	87	123	107
95TH......................................GM......	151		56	61	95	112	112	149	131	216	141	187	149	155	123	165	136
99TH......................................GM......	245		75	112	153	168	157	262	224	328	205	276	240	284	184	224	224
USED ON ONLY 1 OF 3 DAYS:																	
AVERAGE 1/ ....GM......	163	44	62	75	106	135	126	181	149	223	165	202	163	166	140	193	139
STANDARD DEVIATION........................GM......	107	22	41	43	63	78	73	96	99	139	95	110	105	83	87	116	79
USED ON ONLY 2 OF 3 DAYS:																	
AVERAGE 1/ ....GM......	172	69	61	86	126	148	126	172	159	217	157	206	164	169	134	168	165
STANDARD DEVIATION........................GM......	88	0	28	72	87	71	55	90	71	103	62	94	76	78	55	56	83
USED ON ALL 3 OF 3 DAYS:																	
AVERAGE 1/ ....GM......	200	28	54	91	87	0	149	341	178	309	184	209	176	162	65	131	163
STANDARD DEVIATION........................GM......	149	0	11	38	12	0	81	212	24	267	101	82	77	39	0	56	0
MAXIMUM IN ANY 1 DAY......................GM......	1,792	85	255	448	504	896	504	896	693	1,792	736	1,344	972	552	672	672	448
MAXIMUM OVER 3 DAYS.......................GM......	3,312	130	269	816	816	896	800	1,798	740	3,312	1,460	1,540	1,840	644	672	672	672
QUANTITY CONSUMED PER EATING OCCASION:																	
AVERAGE 1/ ....GM......	162	45	60	77	107	137	125	178	147	217	161	196	159	157	132	169	137
STANDARD DEVIATION........................GM......	104	21	37	50	67	78	71	105	91	140	91	105	97	82	72	85	76
PERCENTILES: 1/																	
5TH.......................................GM......	46		14	23	30	46	43	56	54	68	56	72	56	56	54	56	45
25TH......................................GM......	92		28	46	69	85	84	112	92	113	105	112	92	92	85	96	84
50TH......................................GM......	138		56	70	92	112	112	168	115	184	140	176	138	138	112	161	112
75TH......................................GM......	216		84	92	115	168	149	224	168	276	184	224	184	210	168	224	184
90TH......................................GM......	276		112	112	184	224	224	300	224	368	276	336	271	230	224	276	252
95TH......................................GM......	368		122	168	224	280	252	368	324	448	360	414	336	306	224	368	306
99TH......................................GM......	552		168	252	368	368	448	576	553	673	540	553	540	448	448	360	336
MAXIMUM...................................GM......	1,792	85	255	448	504	896	504	896	693	1,792	736	720	972	552	460	448	336
QUANTITIES NOT SPECIFIED BY USERS: 1/																	
EATING OCCASIONS.........................NUMBER....	498.5	1.6	9.8	22.8	19.9	23.1	23.4	17.5	18.0	66.8	61.7	93.3	91.3	10.6	14.0	11.5	13.2
PROPORTION OF EATING OCCASIONS...........PCT......	4.0	11.6	4.1	4.8	3.9	4.0	3.7	4.0	4.5	4.3	3.6	4.2	3.5	3.0	2.9	6.9	6.0

1/ SEE TABLE NOTES IN APPENDIX.

Source: Pao et al. (1982)

The National Center for Health Statistics also conducted a national dietary survey, the National Health and Nutrition Examination Survey (NHANES II) from 1976-1980. This survey obtained 24-hour dietary recalls from 20,325 individuals. The data base from this survey contains 2,614 food items. This survey was less comprehensive than the NFCS survey, and in most cases the NFCS survey would provide the consumption data necessary.

Several other agencies have modified the NFCS and the NHANES data for their own purposes. OPP has used the NFCS data to provide consumption data as part of their Tolerance Assessment System (USEPA 1984a) as described in Section 2.2. FDA used average values for consumption from the two national surveys in order to provide a basis for sampling in the Total Diet Study and for estimating exposure (USEPA 1983b). They used total food consumption as shown in Table 7. Food consumption data were then reported as an average (from the average of the two surveys) percent of the total diet for the eight age-sex groups. No food was included in the Total Diet study which equaled less than 0.02 percent of the total diet by weight. Table 8 shows an example of the daily intakes for 25-30 year old females.

U.S. EPA (1980a) used the 1965-1966 NFCS data to analyze food consumption habits in terms of home grown vs commercially produced fruits and vegetables. Consumption of fruits and vegetables by non-meat eaters was also examined.

These systems could provide useful consumption data for this methodology. TAS was developed for setting pesticide tolerances, and therefore, the NFCS data had to be converted to raw agricultural commodities. If contamination is thought to occur during the food generation stage, TAS would be the most appropriate system to use. The Total Diet Study, on the other hand, is oriented towards providing consumption data for foods as they are prepared and consumed. These data are based on the NFCS and NHANES data, and would not generally provide additional information. The OTS (USEPA 1980a) data, although limited in scope, would be very useful if exposure through home gardens was of interest.

Another source of food consumption data is USDA (1981, 1985). These data provide average intake per capita for a number of food groups. No subpopulations by age or location are considered. This report may, however, contain information on some foods or processing methods not included in NFCS. Table 3 summarized data on consumption of fruit and vegetables from this source.

Section 2.1 describes the ORP dietary exposure assessment methods. The consumption patterns developed for this system are specific to airborne radionuclides and are based on very general food groups. However, these consumption data may be used if airborne contamination is expected, and a great degree of food specificity is not necessary.

One major inadequacy in the consumption pattern data sources discussed above is that they do not consider consumption patterns in different areas of the country aside from the four census regions,

TABLE 7

AVERAGE DAILY INTAKE OF FOOD AND DRINKING WATER FOR SPECIFIED AGE-SEX GROUPS (gms/day)[34]

Age-sex Group Average Daily (grams)	6-11 Months	2 Years	14-16 Year Females	14-16 Year Males	25-30 Year Females	25-30 Year Males	60-65 Year Females	60-65 Year Males
Intake of food*	1071	1182	1515	2109	1777	2590	1711	2149
Intake of water†	150	321	432	548	399	512	546	581
Total intake of food and water‡	1221 (1263)	1503 (1523)	1947 (1954)	2657 (2677)	2176 (2173)	3102 (3075)	2257 (2259)	2730 (2690)

* Average of the daily intake from USDA data and HANES data.

† Derived from the USDA questionnaire regarding consumption in water of cups on previous day.

‡ Due to aggregation summation, rounding of values, omission of several food items from the original NHANES and NFCS data bases, and conversion of same dry weight values to as consumed weights, the daily gram intakes obtained by summing the amounts for 234 foods (shown in parentheses) differs slightly from the values shown here.

Source: Pennington (1981) as cited in USEPA 1983b

TABLE 8 FOOD CONSUMPTION

AGE-SEX GROUP - 25 TO 30 YEAR-OLD FEMALES

Average NHANES grams/day - 1938
Average NFCS grams/day - 1615
Average of NHANES and NFCS grams/day - 1777

Food	NHANES (%)	NFCS (%)	NHANES (g)	NFCS (g)	Average (g)	Average (%)
001 Whole milk	5.310	6.569	102.908	106.059	104.484	5.880
002 Lowfat milk, 2%	3.381	2.506	65.524	40.458	52.991	2.982
003 Chocolate milk	.332	.888	6.434	14.334	10.384	.584
004 Skim milk	.816	.880	15.814	14.206	15.010	.845
005 Buttermilk	.108	.011	2.093	.179	1.136	.064
006 Yogurt, plain	.172	.104	3.333	1.682	2.508	.141
007 Chocolate milkshake	.074	.298	1.434	4.816	3.125	.176
008 Evaporated milk	.033	.013	.640	.217	.428	.024
009 Yogurt, strawberry	.118	.242	2.287	3.905	3.096	.174
010 American cheese	.358	.369	6.938	5.957	6.448	.363
011 Cottage cheese, 4%	.189	.355	3.663	5.734	4.698	.264
012 Cheddar cheese	.287	.335	5.562	5.402	5.482	.309
013 Ground beef	.788	1.112	15.271	17.947	16.609	.935
014 Beef chuck roast	.521	.738	10.097	11.911	11.004	.619
015 Beef round steak	.059	.113	1.143	1.831	1.487	.084
016 Beef loin steak	.706	1.063	13.682	17.171	15.427	.868
017 Pork ham	.410	.361	7.946	5.821	6.883	.387
018 Pork chop	.270	.402	5.233	6.483	5.858	.330
019 Pork sausage	.094	.249	1.822	4.019	2.920	.164
020 Pork bacon	.075	.167	1.454	2.701	2.077	.117
021 Pork roast	.140	.177	2.713	2.859	2.786	.157
022 Lamb chop	.100	.050	1.938	.810	1.374	.077
023 Veal cutlet	.089	.060	1.725	.965	1.345	.076
024 Chicken, fried	.416	.615	8.062	9.926	8.994	.506
025 Chicken, roasted	.408	.714	7.907	11.531	9.719	.547
026 Turkey, roasted	.010	.170	.194	2.750	1.472	.083
027 Liver, fried	.293	.111	5.678	1.797	3.738	.210
028 Frankfurters	.253	.344	4.903	5.560	5.232	.294
029 Bologna	.223	.402	4.322	6.492	5.407	.304
030 Salami	.033	.034	.640	.546	.593	.033
031 Cod, baked	.340	.364	6.589	5.877	6.233	.351
032 Tuna, canned in oil	.200	.287	3.876	4.630	4.253	.239
033 Shrimp, fried	.138	.163	2.674	2.636	2.655	.149
034 Fish sticks, frozen	.076	.125	1.473	2.011	1.742	.098

TABLE 8 FOOD CONSUMPTION

AGE-SEX GROUP - 25 TO 30 YEAR-OLD FEMALES (continued)

	Food	NHANES (%)	NFCS (%)	NHANES (g)	NFCS (g)	Average (g)	Average (%)
035	Eggs, scrambled	.389	.745	7.539	12.028	9.783	.551
036	Eggs, fried	.343	.336	6.647	5.425	6.036	.340
037	Eggs, boiled	.208	.339	4.031	5.470	4.751	.267
038	Pinto beans	.492	.379	9.535	6.117	7.826	.440
039	Pork and beans, canned	.178	.469	3.450	7.569	5.509	.310
040	Cowpeas	.066	.128	1.279	2.059	1.669	.094
041	Limas, mature	.005	.045	.097	.721	.409	.023
042	Limas, immature	.063	.083	1.221	1.344	1.282	.072
043	Navy beans	.038	.042	.736	.684	.710	.040
044	Red beans	.054	.108	1.047	1.745	1.396	.079
045	Peas, canned	.237	.374	4.593	6.045	5.319	.299
046	Peas, frozen	.124	.058	2.403	.939	1.671	.094
047	Peanut butter	.054	.086	1.047	1.381	1.214	.068
048	Peanuts	.039	.044	.756	.705	.731	.041
049	Pecans	.078	.026	1.512	.416	.964	.054
050	White rice	.784	1.028	15.194	16.595	15.895	.895
051	Oatmeal	.216	.283	4.186	4.574	4.380	.247
052	Farina	.085	.136	1.647	2.194	1.921	.108
053	Corn grits	.124	.239	2.403	3.856	3.130	.176
054	Corn, fresh/frozen	.253	.424	4.903	6.846	5.875	.331
055	Corn, canned	.150	.125	2.907	2.012	2.460	.139
056	Corn, creamed style, canned	.066	.121	1.279	1.951	1.615	.091
057	Popcorn	.147	.033	2.849	.531	1.690	.095
058	White bread	1.883	2.004	36.493	32.356	34.424	1.937
059	White rolls	.639	.478	12.384	7.726	10.055	.566
060	Cornbread	.185	.257	3.585	4.152	3.869	.218
061	Biscuits	.156	.192	3.023	3.102	3.063	.172
062	Whole wheat bread	.166	.318	3.217	5.139	4.178	.235
063	Tortilla, flour	.148	.108	2.868	1.744	2.306	.130
064	Rye bread	.108	.082	2.093	1.328	1.711	.096
065	Muffins	.070	.033	1.357	.537	.947	.053
066	Saltines	.207	.183	4.012	2.952	3.482	.196
067	Corn chips	.045	.046	.872	.745	.809	.046
068	Pancakes	.212	.301	4.109	4.855	4.482	.252
069	Noodles	.089	.124	1.725	1.994	1.859	.105
070	Macaroni	.223	.290	4.322	6.302	5.312	.299

TABLE 8 FOOD CONSUMPTION

AGE-SEX GROUP - 25 to 30-YEAR-OLD FEMALES (continued)

Food	NHANES (%)	NFCS (%)	NHANES (g)	NFCS (g)	Average (g)	Average (%)
071 Cornflakes	.071	.076	1.473	1.224	1.348	.076
072 Fruit type cereal	.015	.014	.291	.230	.260	.015
073 Shredded wheat	.073	.100	1.415	1.615	1.515	.085
074 Raisin bran	.051	.091	.988	1.473	1.231	.069
075 Crisped rice	.045	.042	.872	.680	.776	.044
076 Granola	.045	.019	.872	.301	.587	.033
077 Oat ring cereal	.019	.035	.368	.566	.467	.026
078 Apple, raw	.761	.819	14.748	13.221	13.985	.787
079 Orange, raw	.454	.443	8.799	7.150	7.974	.449
080 Banana, raw	.301	.363	5.833	5.865	5.849	.329
081 Watermelon, raw	.237	.195	4.593	3.141	3.867	.218
082 Peach, canned	.102	.175	1.977	2.827	2.402	.135
083 Peach, raw	.186	.252	3.605	4.064	3.834	.216
084 Applesauce, canned	.088	.197	1.705	3.176	2.441	.137
085 Pear, raw	.148	.087	2.868	1.411	2.140	.120
086 Strawberries, raw	.094	.120	1.822	1.942	1.882	.106
087 Fruit cocktail, canned	.245	.191	4.748	3.086	3.917	.220
088 Grapes, raw	.080	.052	1.550	.841	1.196	.067
089 Cantaloupe, raw	.220	.125	4.264	2.013	3.138	.177
090 Pear, canned	.014	.081	.271	1.316	.794	.045
091 Plums, raw	.048	.033	.930	.538	.734	.041
092 Grapefruit, raw	.476	.197	9.225	3.177	6.201	.349
093 Pineapple, canned	.084	.072	1.628	1.164	1.396	.079
094 Cherries, raw	.025	.043	.485	.699	.592	.033
095 Raisins, dried	.006	.025	.116	.398	.257	.015
096 Prunes, dried	.004	.006	.078	.104	.091	.005
097 Avocado, raw	.091	.053	1.764	.859	1.311	.074
098 Orange juice, frozen	2.938	2.733	56.938	44.123	50.531	2.844
099 Apple juice, canned	.358	.370	6.938	5.969	6.454	.363
100 Grapefruit juice, frozen	.428	.326	8.295	5.258	6.776	.381
101 Grape juice, canned	.190	.335	3.682	5.411	4.547	.256
102 Pineapple juice, canned	.060	.081	1.163	1.309	1.236	.070
103 Prune juice, bottled	.000	.020	.000	.328	.164	.009
104 Orange drink, canned	.902	.878	17.481	14.171	15.826	.891
105 Lemonade, frozen	.396	.626	7.675	10.106	8.890	.500
106 Spinach, canned	.030	.067	.581	1.081	.831	.047
107 Spinach, fresh/frozen boiled	.130	.152	2.519	2.450	2.485	.140
108 Collards, boiled	.039	.065	.756	1.051	.903	.051
109 Lettuce	1.135	1.554	21.996	25.084	23.540	1.325
110 Cabbage, boiled	.166	.177	3.217	2.854	3.036	.171
111 Coleslaw	.108	.170	2.093	2.750	2.422	.136
112 Sauerkraut, canned	.040	.033	.775	.536	.656	.037

TABLE 8 FOOD CONSUMPTION

AGE-SEX GROUP - 25 TO 30 YEAR-OLD FEMALES (continued)

	Food	NHANES (%)	NFCS (%)	NHANES (g)	NFCS (g)	Average (g)	Average (%)
153	Pork chow mein	.085	.372	1.647	6.009	3.824	.215
154	Frozen dinnner, fried chicken	.062	.099	1.202	1.597	1.399	.079
155	Bouillon	.295	.639	5.717	10.309	8.013	.451
156	Chicken noodle soup	.219	.616	4.244	9.940	7.092	.399
157	Creamed tomato soup	.326	.953	6.319	15.390	10.854	.611
158	Vegetable beef soup	.512	.133	9.923	1.817	5.870	.330
159	Gravy	.144	.284	2.791	4.593	3.692	.208
160	White sauce	.091	.012	1.764	.194	.979	.055
161	Dill pickles	.051	.101	.988	1.629	1.309	.074
162	Margarine	.220	.193	4.264	3.119	3.691	.208
163	Salad dressing, Italian	.289	.345	5.601	5.576	5.558	.315
164	Butter	.136	.140	2.636	2.254	2.445	.138
165	Corn oil	.127	.016	2.461	.263	1.362	.077
166	Mayonnaise	.054	.098	1.047	1.581	1.314	.074
167	Cream, 1/2 and 1/2	.097	.102	1.880	1.647	1.763	.099
168	Cream substitute	.072	.033	1.395	.529	.962	.054
169	Sugar	.337	.270	6.531	4.365	5.448	.307
170	Corn syrup	.091	.165	1.764	2.662	2.213	.125
171	Grape jelly	.149	.095	2.888	1.535	2.211	.124
172	Honey	.026	.029	.504	.475	.489	.028
173	Catsup	.095	.092	1.841	1.482	1.662	.094
174	Ice cream, chocolate	.497	.563	9.632	9.087	9.359	.527
175	Pudding, chocolate	.133	.171	2.578	2.766	2.672	.150
176	Ice cream sandwich	.030	.046	.581	.741	.661	.037
177	Ice milk, vanilla	.149	.056	2.888	.911	1.899	.107
178	Chocolate cake and chocolate icing	.190	.186	3.682	3.002	3.342	.188
179	Yellow cake and white icing	.331	.295	6.415	4.763	5.589	.315
180	Coffeecake	.034	.051	.659	.829	.744	.042
181	Doughnut	.259	.146	5.019	2.362	3.691	.208
192	Danish pastry	.099	.133	1.919	2.140	2.030	.144
183	Chocolate chip cookies	.255	.159	4.942	2.561	3.751	.211
184	Sandwich cookies	.118	.063	2.287	1.010	1.648	.093
185	Apple pie	.285	.264	5.523	4.269	4.896	.276
186	Pumpkin pie	.168	.208	3.256	3.351	3.303	.186
187	Chocolate candy	.212	.092	4.109	1.486	2.797	.157
188	Carmel candy	.076	.111	1.473	1.793	1.633	.092
189	Chocolate powder	.079	.205	1.531	.401	.966	.054
190	Gelatin dessert, strawberry	.154	.229	2.985	3.701	3.343	.188

TABLE 8 FOOD CONSUMPTION

AGE-SEX GROUP - 25 TO 30 YEAR-OLD FEMALES (continued)

	Food	NHANES (%)	NFCS (%)	NHANES (g)	NFCS (g)	Average (g)	Average (%)
191	Soda, cola	7.420	7.548	143.800	121.878	132.839	7.476
192	Soda, lemon-lime	2.927	1.642	56.725	26.518	41.622	2.342
193	Soft drink, cherry	2.250	1.324	43.605	21.375	32.490	1.828
194	Soda, low calorie, cola	3.346	2.697	64.846	43.546	54.196	3.050
195	Coffee beverage	18.227	13.230	353.239	213.615	283.427	15.950
196	Coffee beverage, decaffeinated	1.031	.900	19.981	14.527	17.254	.971
197	Tea beverage	9.037	9.385	175.137	151.528	163.333	9.195
198	Beer	2.481	1.307	48.082	21.100	34.591	1.947
199	Wine	.775	.547	15.020	8.830	11.925	.671
200	Whisky	.229	.337	4.438	5.433	4.936	.278
201	Water	--	--	--	--	--	--

Source: U.S. EPA 1983b

northeast, north central, south, and west; and the three urbanizations, central city, suburban, and non-metropolitan. In addition, specific subpopulations (e.g., vegetarians) are not generally considered. While these variations would be reflected in the distribution of intakes, any geographic patterns would not be differentiated. For example, consumption of home grown produce or locally caught fish may be important in very localized areas. Of interest in this regard is a report by Puffer et al. (1982), which examined the fish consumption rates by fishermen and their families in the metropolitan Los Angeles area. Table 9 shows the distribution of consumption reported in this study. These data show an interesting pattern. The median consumption of fish by the sport fishermen is somewhat lower than that by the users among the U.S. population (those persons reporting consumption of fish). Fish consumption at the high end of the range, however, is much higher for the sport fishermen. Similar studies have been conducted in a few other areas, e.g., Puget Sound (Pierce et al. 1981) and the Mississippi Delta area (USEPA 1982). Such examples show the potential variation in consumption patterns by different subpopulation groups. If specific information not available from the National Surveys is needed, a search of the literature may provide more specific data. Unfortunately, such information is rarely available, and the national data must be used directly or modified by some assumptions about specific food items or areas of the country.

3.2.3. Population Data

The size of the population is determined to some extent by the amount of food potentially contaminated. Appendix A describes methods for determining the quantity of food contaminated. Numerous sources of data are available for assessing such quantities:

- Census of Agriculture (USDOC 1981)

  - areas where foods are grown; extensive statistics on number of head of stock or acres of crop production by county for entire U.S.; livestock and poultry--numbers/county; crops--acres/county;location and production of fish farms (not commercial or sport fishing acres)

- National Marine Fisheries Service (NMFS) of NOAA (NMFS 1980a) Fishery Statistics of the United States 1976

  - Commercial fisheries statistics

- National Marine Fisheries Service. Fisheries of the United States 1982. (NMFS 1983)

  - U.S. Commercial landings by state, and at about 120 major U.S. ports, in pounds and dollars

- National Marine Fisheries Service. Marine Recreational Fishery Statistics (NMFS 1980b)

TABLE 9

FISH CONSUMPTION PATTERNS FOR SPORT FISHERMEN AS COMPARED TO THE U.S. POPULATION

	Consumption Rate (g/day/person)*	
Percentile	LA Sport Fishermen	Nationwide USDA Survey
5	2.3	11
25	11.9	27
50	36.9	47
75	100.3	80
90	244.8	128
95	338.8	165

* The USDA data are for males 19-34 since this was the age group most comparable to the Los Angeles study population. Fish was consumed at least once in three days. In the LA study, 68% of the respondents reported eating fish one time per week or more. The median daily consumption was 127.2 g/day for frequent eaters (3-7 times/week) and 27.2 g/day for infrequent eaters.

Source: Pao et al. 1982; Puffer et al. 1981

  - Summaries of fish caught by state and by various other characteristics

- AGDATC and AGDATG (Baes et al. 1985). Contact: B.L. McGill, Oak Ridge National Laboratories, Oak Ridge, TN 37831 (615-574-6176).

  - Two agricultural data libraries containing agricultural production for vegetables and produce, livestock and livestock feeds. Intended for use in exposure assessment, specifically for radionuclides. Data by county or long/lat grid cell.

- Office of Drinking Water, The Federal Reporting Data System -- Public Water Systems. Contact: Mr. Avrum W. Marks, USEPA, Office of Drinking Water (202-382-5513).

  - Database documents public water supplies by county or city, giving source information, population served, and treatment techniques used.

- The Chilton Company (1981) Directory of U.S. Food and Beverage Plants

  - Lists all food and beverage plants within a county, products produced, peak employment; no volume of production

- Trinet, Inc. (Economic Information Systems, Inc.)

  - Trinet market share data base (% sales) for each plant within a given SIC category. Contact: Trinet, Inc. 9 Campus Drive, Parsippany, NJ 07054.

- Census of Manufacturers, USDOC (1980)

  - Total volume of shipments for the U.S. within the SIC code

Data addressing population sizes (or users) for the U.S. are contained in USDA (1983) as described above. In addition, if the population exposed is defined geographically, the total population in an area can be obtained from U.S. Census data as described in Dixon et al. (1985). In some cases, it may be useful to determine the total population in a specific area and then to estimate the user population using the national or regional data developed by USDA (1983).

4.0 SUMMARY AND EXAMPLE

The previous section has described a step-by-step approach to assessing dietary intake. This approach uses available monitoring information, but may be supplemented by a pathways approach which is intended to identify the more significant situations of food contact. This seems like a straightforward procedure, but in practice, many unexpected situations may arise. The best way to further describe the approach is by example. This section therefore describes a hypothetical application of the step-by-step approach using the chemical benzanthrone.

Step 1 Determine the Scope of the Assessment

Benzanthrone is an existing chemical, primarily used as an intermediate. Therefore, monitoring data are expected to be scarce and estimation of contamination resulting from significant pathways will be conducted when possible. Mean residue data and consumption data will be used. The assessment will be on a national basis.

Step 2 Collect Available Residue Data

No residue data were available for benzanthrone. For the purpose of this example, data on benz(a)anthracene were used as shown in Table 10. It is not suggested that these chemicals are structurally similiar. The monitoring data was used to show how such data could be incorporated into an analysis. These residues are generally attributed to formation during cooking. In such a case, the pathways approach cannot be used to compare predicted results with measured results since residues produced during cooking will not be predicted in the pathways approach. These measured values are included here to show the associated consumption patterns and the populations exposed as compared to the consumption patterns and populations exposed for the predicted exposure pathways.

Step 3 Pathways Approach

The detailed application of the pathways approach for benzanthrone is described in Appendix C. The results of this method are shown in Table 11.

Step 4 Estimate Concentrations in Food

Appendix C details the quantification methods used for estimating concentrations of benzanthrone in food. The results are shown in Table 4-2.

Step 5 Compile Food Concentration Data

In Step 5, the available concentration data should be compiled by exposure group as well as by food group. Table 12 shows a hypothetical summary for benzanthrone.

TABLE 10

LEVELS OF BENZ(A)ANTHRACENE IN FOOD

Food Item	Average Concentration (ug/kg)
Charcoal-Broiled Steak	3
Smoked Pork	3
Smoked Sausage	0.2
Smoked Fish	1
Oil	1

Source: Perwak et al. (1981b)

TABLE 11

SIGNIFICANT PATHWAYS OF CONTAMINATION AND ESTIMATED CONCENTRATIONS --BENZANTHRONE

Source of Human Exposure	Contamination Pathway	Estimated Concentration (ug/kg)
Meat	Ingestion of Drinking Water	0.045 (beef)
Beef Dairy Hogs and Pigs Sheep and Lamb Poultry		
Fish	Absorption From Water	4500
Food- Post Harvest	Absorption/Addition of Water used in Processing	1 fruits and vegetables
		10 beverages

Source: Appendix C

TABLE 12

HYPOTHETICAL COMPILATION OF FOOD CONCENTRATION DATA AND FOOD CONSUMPTION - BENZANTHRONE

Exposure Group	Food Groups	Mean Food Concentration (ug/kg)	Average Consumption g/day
General Population	Meat		
	Charcoal-broiled steak	3[a]	2[c]
	Smoked pork	3[a]	1[d]
	Smoked sausage	0.2[a]	1[e]
	Fish/Shellfish		
	Smoked fish	1[a]	0.1[f]
	Oil	1[a]	14[g]
Persons consuming food generated or processed near production facilities	Meat		
	Beef	0.045[b]	54[h]
	Fish/Shellfish	4500[b]	11[h]
	Vegetables	1[b]	201[h]
	Fruit	1[b]	72[h]
	Beverages	10[b]	604[h]

a Measured concentration for benz[a]anthracene
b Estimated concentration for benzanthrone
c Consumption of beef - 54 g/day (USDA 1980). Assumed 15% charcoal broiled, 20% steak
d Consumption of pork - 20 g/day (USDA 1980). Assumed 5% smoked
e Consumption of sausage - 20 g/day (USDA 1980). Assumed 5% smoked
f Consumption of fish/shellfish - 11 g/day (USDA 1980). Assumed 1% smoked.
g USDA (1980)
h USDA (1980). Assumes all consumption comes from contaminated area.

Step 6 Collect Appropriate Consumption Data

Table 12 also shows average U.S. consumption data for the foods included in the assessment. This table shows that assumptions are commonly made about the nature of the food in a particular group. In the example, assumptions were made about the portion of the total consumption that was charcoal-broiled or smoked. For the population exposed to food contaminated in the area of the production releases, it was assumed that their total consumption of these items was from the contaminated area. This implies a worst case in terms of exposure, but a minimum number of persons exposed.

Step 7 Estimate Individual Exposure

With the information in Table 12, individual exposure can be calculated using Equation 3-1. The hypothetical results are summarized in Table 13. Exposure in this hypothetical example is greater to those people consuming food contaminated in the vicinity of benzanthrone production facilities than to those consuming charcoal-broiled or smoked meats (using the data for benz-(a)anthracene). It should always be noted that such a conclusion is based upon a long series of estimation procedures in the pathways approach, from the fate processes to the food contamination situations, with uncertainties associated with each step. On the other hand, limited monitoring data must sometimes be used to represent average U.S. concentrations. In most cases, however, the use of monitoring data is preferable, if available.

Step 8 Estimate Population Exposed

In this example, two populations were identified. One population was persons exposed to this compound in meats that are charcoal-broiled or smoked. The population size must be considered on a food-by-food basis. For example, Pao et al. (1982) showed that 67.3% of the individuals in the food consumption survey consumed beef at least once in three days. These persons are designated as the users and are the exposed population (67.3% of the U.S. population) for beef. Similarly 49.9% of the population consumed pork, and 13.5% of the population consumed sausage.

The population sizes of the second group (food contaminated near the production facility) are more difficult to quantify. Again, the sizes should be considered on a food-by-food basis. The actual sizes are dependent upon the amount of each food type contaminated and the distribution patterns for each. In this example, the amount of food contaminated was not quantified, but benzanthrone production is limited to eight sites. In addition, it was assumed that the exposed population received 100% of their consumption of the identified foods from the contaminated area. Considering these assumptions, the exposed population would be quite small.

TABLE 13

SUMMARY OF HYPOTHETICAL INDIVIDUAL DIETARY EXPOSURE -- BENZANTHRONE

Exposure Group	Food Group	Exposure (ug/day)
General Population	Meat	0.009
	Fish/Shellfish	0.0001
	Oil	0.01
	Total	0.02
Persons Consuming Food Generated or Processed near Production Facilities	Meat	0.002
	Fish/Shellfish	50
	Vegetables	0.2
	Fruit	0.07
	Beverages	6
	Exposure to General Population	0.02
	Total	60

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APPENDIX A
PATHWAYS OF FOOD CONTAMINATION

A.1 INTRODUCTION

There are many pathways by which a chemical can find its way into food. Not all of these pathways are equally significant. The main objective of this appendix is to present a methodology that can be used to identify the most significant pathways based on chemical properties, use characteristics, and chemical release characteristics.

A.2 PATHWAYS OF FOOD CONTAMINATION

Figure 4 showed the potential contamination pathways of a pollutant to food. Besides the pathways shown, pathways due to accidents or misuse should also be considered. There are two types of pathways by which food may become contaminated, direct and indirect pathways. Indirect pathways involve release of a pollutant to another medium, while direct pathways involve the direct addition of the chemical to food, for example, food additives or pesticides. Table 14 shows the food chain access points during food generation stages (pre-harvest) by food groups. This table shows the points and the nature of media contact with food (indirect pathways) and any additions that may occur (direct pathways). Table 15 shows the food chain access points in the food processing and consumption stages (post-harvest). In this table, the points of contact are described by step, rather than by food groups, since the type of contact does not depend as much on the food group as on the step. Table 15 also eliminates soil/sediment as a potential pathway, and contact surfaces are added for the post-harvest stages. Table 16 expands on the nature of these access points for food in the post-harvest stages. Table 17 relates the food chain access points to food contamination pathways; these pathways are used as a starting point for Appendix B, Quantitative Methods. Tables 14, 15, 16 and 17 show where contaminants can enter food, by food group or by processing step. While this information is useful in understanding the scope of the problem, it does not provide any insight into which pathways are potentially important for a given chemical. The important pathways can be identified only by relating characteristics of the chemical and its uses to pathways.

A.3 SIGNIFICANT PATHWAYS IDENTIFICATION METHODOLOGY

Figure 5 shows the Pathways Identification Methodology, which can be used to identify the most significant pathways for the chemical of concern. For a particular chemical, the first step is to identify all the situations of release from the production and use characteristics of the chemical. The production of the chemical as a degradation product or in treatment processes should also be considered. The first result of this is the identification of all the situations of direct contact, i.e., direct addition of the chemical to food at some

TABLE 14 FOOD CHAIN ACCESS POINTS
FOOD GENERATION STAGES (PRE-HARVEST)

	ANIMAL				VEGETABLE		OTHER MATERIALS
	Meat	Poultry	Dairy Cows	Fish and Seafood Products	Fruit Vegetable Nuts	Marine Plants	(Natural Raw Materials & Synthetics)
Air	Ambient Air in grazing areas or pens	Ambient Air in poultry houses	Ambient Air in grazing areas enclosed area	---	Ambient Air	---	Ambient Air
Water	Drinking water	Drinking water	Drinking water	Ambient water contacted	Rainwater, ambient water used for irrigation	Ambient Water contacted	Ambient Water
Soil/ Sediment	Soil in grazing area or enclosed area, bedding	Litter	Soil in grazing area or enclosed area, bedding	Sediment in area	Soil in growing area	Sediment in area	Soil/Sediment if mined
Addition	Growth promotor, antibiotics, feed	Growth promotor, antibiotics, feed	Growth promotor, antibiotics, feed	Growth promotors, antibiotics, feed for cultured products	Pesticides, fertilizers soil additives	Pesticides, feed for cultured plants	Mining aids

TABLE 15 FOOD CHAIN ACCESS POINTS
FOOD PROCESSING/CONSUMPTION STAGES (POST HARVEST)

MEDIA	HARVEST	STORAGE	RAW MATERIAL CONVERSION	FORMULATION TECHNIQUES	PACKAGING	PRESERVATION TECHNIQUES	STORAGE AND DISTRIBUTION (perishable and shelf-stable)	PREPARATION AND CONSUMPTION
Air	Ambient Air	air of storage area	air of preparation area	air of preparation room, compressed air	compressed air, modified atmosphere		air in warehouse vehicle retail store refrigerator/freezer	air of preparation area
Water			wash water	process water, steam (boiler water addition)	container rinse	process water, steam		wash water cooking water
Contact Surface	Harvest equipment	storage surface	food contact surfaces	food contact surfaces	packaging material	food contact surfaces	packaging material	cooking utensils
Addition	"Soil", maintenance compounds, harvesting aids	pesticides, storage aids, maintenance and sanitation compounds	cleaning and sanitation compounds	intentional and incidental addition, process aids	sanitizers, chemical sterilants, tailored atmosphere (CO_2, N_2, specialty)	preservatives	spills cross contamination	cross contamination

TABLE 16 . POST HARVEST FOOD CHAIN ACCESS POINTS

HARVEST/SLAUGHTER	
Air	During the harvest process, air is blown onto fruits and vegetables to separate them; they are also separated by gravimetric techniques. Meat and poultry are exposed to the ambient air during transportation to slaughter (usually in trucks) and in the area in which they are slaughtered. Additionally, hogs are exposed to carbon dioxide to desensitize them to pain before slaughter.
Water	Some field crops are harvested with the aid of water for washing (e.g., cranberries). There exists, in this situation, a potential for both soil and water contamination. Animal carcasses which will be processed for meat consumption are washed once they have been eviscerated. Hogs, however, are "scalded" following bleeding, by being immersed in water at 140° F.
STORAGE	
Air	Potential exists for exposure to contaminated air during storage of harvested fruits and vegetables. Animal carcasses, once they have been eviscerated, are refrigerated for up to 48 hours.
Other	There is some likelihood that crops will come into contact with surfaces of treated wood used in storage areas, as well as pesticides and sanitation compounds sprayed in these areas.
RAW MATERIAL CONVERSION	
Air	Field crops are potentially exposed to air contaminants in the area in which they are processed; this is also true of meat and dairy products which are aged or cured.
Water	Exposure to contaminated water during raw material conversion of crops, meat, and dairy products is a possibility during food processing.
Other	Other sources of exposure during post-harvest processing are cutting, and the use of waxes and colorings and potentially contaminated additives in food processing.

TABLE 16 POST-HARVEST FOOD CHAIN ACCESS POINTS
(CONTINUED)

FORMULATION TECHNIQUES	
Air	The use of compressed air in food preparation (e.g., steaming and blanching) is a potential pathway for contamination of foods, both meat and vegetable.
Water	Contaminated water used during food formulation/ preparation is a potential source of contamination. Additionally, surfactants, lubricants, and residual sanitizers can result in contamination during food processing.
Packaging	The air, water, and plastics used in food packages are also potential sources of food contamination.
PRESERVATION TECHNIQUES	
Water	Potential pathways of contamination in this area are tainted cooking media, and contact with surfaces which have been washed with contaminated water.
Air	Liquid carbon dioxide, liquid nitrogen, and air used in the dehydration process of crop and meat products represent potential sources of contamination.

TABLE 17. PATHWAY IDENTIFICATION FOR INDIRECT ROUTES OF CONTAMINATION

TYPE OF RELEASE	Food Chain Access	Pathways of Contamination
Release to Ambient Air		
FOOD GENERATION		
	Meat Beef Dairy Cows Hogs and Pigs Sheep and Lamb Poultry	-Inhalation -Absorption of vapors or deposited particulates
	Fish/Shellfish	-Absorption from water where deposition has occurred
	Plants Field Crops Vegetables Berries/Orchard Fruits	-Absorption of vapors or deposited particulates -Uptake from soil where deposited has occurred
FOOD STORAGE/PROCESSING/PREPARATION	Food in Post-Harvest Stages	-Absorption of compound that has infilrated the indoor environment
WATER SUPPLIES	Meat	-Ingestion of water where deposition has occurred
	Plants (irrigation water)	-Uptake from irrigation water where deposition has occurred
FEED GENERATION	Field Crops	-Ingestion of food by livestock and poultry grown where deposition on soil has occurred

TABLE 17. PATHWAY IDENTIFICATION FOR INDIRECT ROUTES OF CONTAMINATION (continued)

TYPE OF RELEASE	Food Chain Access	Pathways of Contamination
Release to Ambient Water		
WATER SUPPLIES		
	Meat Beef Dairy Cows Hogs and Pigs Sheep and Lamb Poultry	-Ingestion of drinking water -Absorption from water used for cooling animals
	Commercial or sport fishing/ shellfishing	-Absorption from water -Consumption of food that has sorbed or ingested pollutants
	Food in post-harvest stages	-Absorption from water used in processing or preparation
	Plants Field crops Vegetables Berries Orchard Fruits	-Uptake from irrigation water
FOOD PROCESSING/PREPARATION	Food in post-harvest stages	-Absorption from water used in processing or preparation -Water used as a component of item
Release to Soil (landfilling, land spreading, solid waste disposal)		
FOOD GENERATION	Meat Beef Dairy cows Hogs and Pigs Sheep and Lamb Poultry	-Absorption from soil via direct contact

TABLE 17. PATHWAY IDENTIFICATION FOR INDIRECT ROUTES OF CONTAMINATION (continued)

TYPE OF RELEASE	Food Chain Access	Pathways of Contamination
Release to Soil (continued)	Fish/Shellfish	-Absorption from water contaminated via runoff or groundwater flow from contaminated area
	Plants Field crops Vegetables Berries/orchard fruits	-Absorption form soil/groundwater from contaminated area
FOOD PROCESSING AND PREPARATION	Food in post-harvest stages	-Absorption from processing water contamination by disposal (groundwater or surface) -Water (contaminated by disposal area) used as component of food item
WATER SUPPLIES		
	Meat	-Ingestion of groundwater contaminated from disposal area
	Plants (irrigation water)	-Uptake from irrigation water which has been contaminated
FEED GENERATION		
	Field crops	-Ingestion of food grown on contaminated soil
Release to Indoor Air		
FOOD STORAGE/PROCESSING/PREPARATION	Food in post-harvest stages	-Absorption/adsorption by food
Release to Water in Storage distribution and use		
FOOD STORAGE/PROCESSING/PREPARATION	Food in post-harvest stages	-Absorption/adsorption by food -Water used as a component of food item.

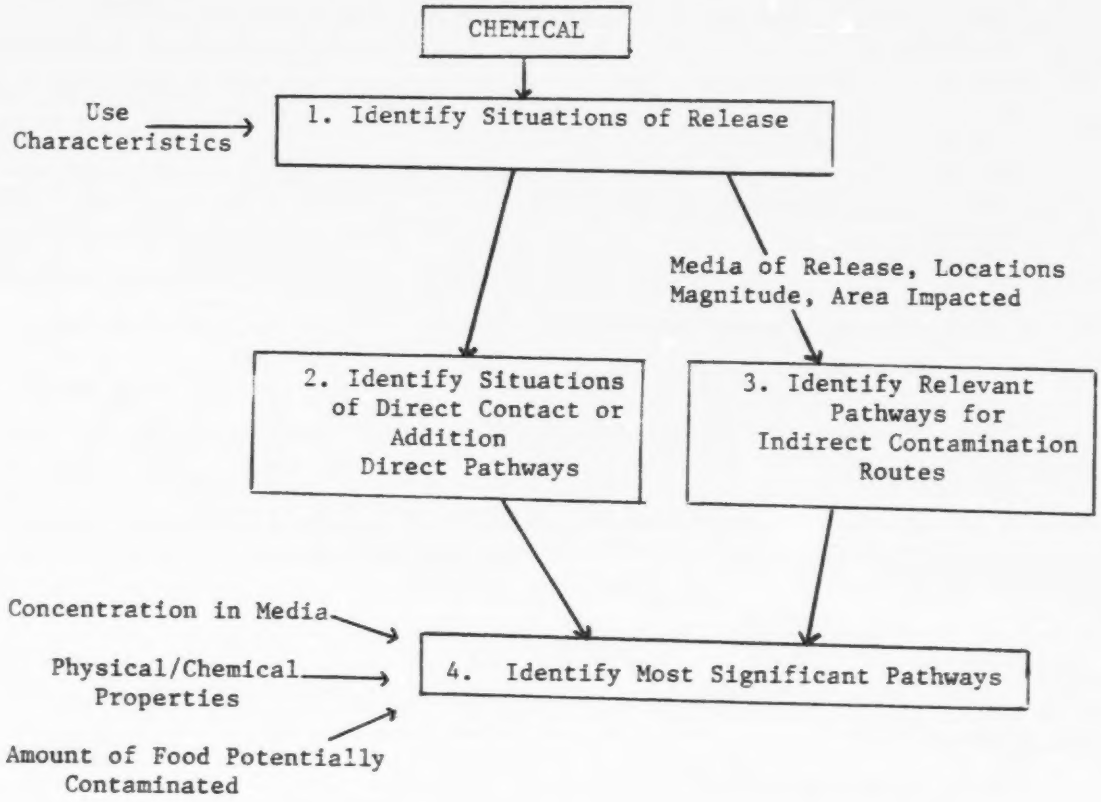

CHEMICAL
Use Characteristics
1. Identify Situations of Release
Media of Release, Locations Magnitude, Area Impacted
2. Identify Situations of Direct Contact or Addition Direct Pathways
3. Identify Relevant Pathways for Indirect Contamination Routes
Concentration in Media
Physical/Chemical Properties
Amount of Food Potentially Contaminated
4. Identify Most Significant Pathways

FIGURE 5 PATHWAYS IDENTIFICATION METHODOLOGY

stage of food production and processing. The second result of the first step involves collecting information regarding the media of release, locations, magnitude of release, and the area impacted. This information allows the identification, using Table 17, of the relevant pathways for indirect contamination routes. From the relevant direct and indirect pathways, the most significant pathways may then be identified using such considerations as the concentration in the media, the physical/chemical properties, and the amount of food potentially contaminated. With this small number of pathways, quantitative methods as described in Appendix B may be used, if necessary, to estimate concentrations found in food from these pathways.

A.3.1 Situations of Release (Step 1)

The intent of Step 1 of the methodology is to identify situations in which the chemical is released to or formed in the environment. The production and use characteristics of the chemical serve as input to this step. The expected outcome of this step is as much detail as possible on the locations and media of releases, magnitude of the releases, and the expected area impacted. A companion volume to this report contains a discussion of sources and releases (Freed et al. 1985).

The extent to which the releases of the compounds can be elaborated will greatly affect the user's ability to limit the scope of the food methodology. If situations of release can be identified, the consideration of pathways can be limited and more definitive.

A.3.2 Situations of Direct Contact (Step 2)

Chemicals may come into direct contact with foods either as additives during formulation of the food product or as processing aids, pesticides, cleaning compounds, sanitizers or other such products used in the production, processing, packaging and distribution of food. All of the above food contact situations are regulated by federal, state, and local laws, rules, and regulations. Each new situation of contact is evaluated on its merit, based first on the functionality of the additive and then on the safety of the use.

The two basic laws regulating food production and processing in the U.S. are the Federal Meat Inspection Act and the Federal Food, Drug, and Cosmetic Act. The latter of these two Acts (laws) provides the basic definitions and regulations regarding the addition of substances to foods. Section 201(s) defines the term "food additive," section 409 addresses the issues of food additive approvals, sections 401, 402, and 403 define the food standards and classes of compliance deviations, and sections 301 to 307 describe the remedies for violations. Additionally, the responsibility for the regulation of compounds such as pesticides and sanitizers is administered by EPA under FIFRA in cooperation with USDA and FDA. Tables 14 to 16 outline many of these use situations.

Lists of the currently regulated food additives are contained in a myriad of titles of the Code of Federal Regulations. Also, some proprietary listing services such as the Food Chemical News Guide and Commerce Clearing House keep abreast of the currently approved and pending (petitioned) uses. Food grade chemicals are generally produced, or segregated, based on purity specifications more stringent than their industrial counterparts. "Food Grade, "U.S.P.", "P.C.C." or other standards generally describe them; their industrial counterparts, however, may contain trace impurities which are quite toxic and underline the seriousness of a possible mislabeling occurrence. Many compounds are also only suitable at specific use levels. At lower or higher levels than the approved usage, or if not used strictly in accordance with approved procedures, they may not function properly or may become very toxic. Thus, the potential for misuse is also a serious concern.

A.3.3 Identification of Relevant Contamination Pathways (Step 3)

Contamination pathways are defined as pathways of pollutant migration from the source to food, including the food chain access point(s). Contamination pathways, as defined previously, are of two basic types: indirect and direct. A chemical has the potential for contaminating food by one, both, or neither of these types of pathways. Direct pathways have been described in Step 2.

For indirect pathways, the major goal is to determine whether the chemical is or could be found in any media contacting food. Table 17 showed the relationship of release characteristics to food chain access points and the pathways of potential contamination. The output of Step 1 is a description of release characteristics of the chemical. This description corresponds to the left column of Table 17. The second column lists all the specific food access points of contact. For each particular release situation, there is a sub-set of possible food access points. The implication of this column is that a fate analysis has been conducted and the distribution of the chemical from the source has been determined. A fate analysis in this context is an assessment of the chemical distribution from the source to various media, and chemical transformations occurring during the distribution. Such an analysis can be conducted using a wide variety of techniques and levels of detail. In general, this distribution can be evaluated either through modeling or through the collection of monitoring data. Methods for conducting such a fate analysis are described in Freed et al. (1985). Once the type of release and the distribution of the chemical has been determined, the points of contact with food items can be evaluated.

For example, if releases to air from production of a particular chemical have been confirmed, a fate analysis will show the extent and level of contamination. The second column in Table 17 can then be used to direct the identification of points of food chain access based primarily on geographical considerations, especially for pathways including food generation areas. If contact is possible, that is, certain foods or food types are generated or processed in the area, the third column indicates the contamination pathways that are possible. The ability to locate areas of release, and thus concentrations of a pollutant in various media, will depend to some extent on the uses. If the use is limited to the production site (e.g., it is used as an intermediate), the locations are likely to be known. If, on the other hand, use is widely distributed, such as with a paint additive, locations are likely to be numerous and geographically disperse. Pathways can sometimes be eliminated on the basis of the nature of the use, i.e., a chemical used as an industrial binder for magnetic tape. In such a case, environmental releases during use are not likely to be in the vicinity of food generation areas, as the chemical would be used indoors, primarily in urban/suburban areas. However, there is some potential for releases to indoor air, and these releases may occur in food processing areas. Releases of this compound from production, could also be in the vicinity of food generation areas. Therefore, the consideration of contamination during food generation stages is limited to the consideration of a few sites. For contamination during food processing, it must first be determined in the fate analysis whether such a compound would be released to the air during use. Then, the potential for this chemical occurring in food storage, processing, or preparation areas can be evaluated.

The identification of relevant contamination pathways can be conducted on several different levels, depending on the specificity of the release characteristics. In this step there is no attempt to prioritize pathways, but simply to eliminate the ones which are clearly impossible based upon expected locations of the chemical in the environment and the locations of food generation, storage, processing, and preparation areas.

The releases to indoor air and to water in storage, distribution, and use (in-plant releases to water used in processing or preparation) are treated somewhat differently than those releases to the ambient environment. This type of release is primarily dependent on the intended use of the compound. The question then is, do releases from such a use have the potential for contacting food in storage, processing, and preparation areas. For example, solvent used in machine degreasing could potentially be used for food processing machinery and may result in releases to air in food storage, processing or preparation areas. Such uses would generally be regulated by FDA, although this may not always be the case.

Table 18 shows chemical applications which may result in releases to indoor air. SRI (1980) contains numerous chemical functions which

TABLE 18

CHEMICAL APPLICATIONS WHICH MAY RESULT IN RELEASES TO INDOOR AIR

Construction

Textiles and Textile Finishing

Apparel and Other Fabricated Textile Products

Lumber and Wood Products

Furniture and Fixtures

Paper and Allied Products

Rubber and Plastic Products

Stone, Clay, Glass, and Concrete Products

Machinery*

Electrical and Electronic Equipment*

*These applications are not likely to be found in food preparation areas, but could be found in food processing areas.

Source: Taken from SRI (1980)

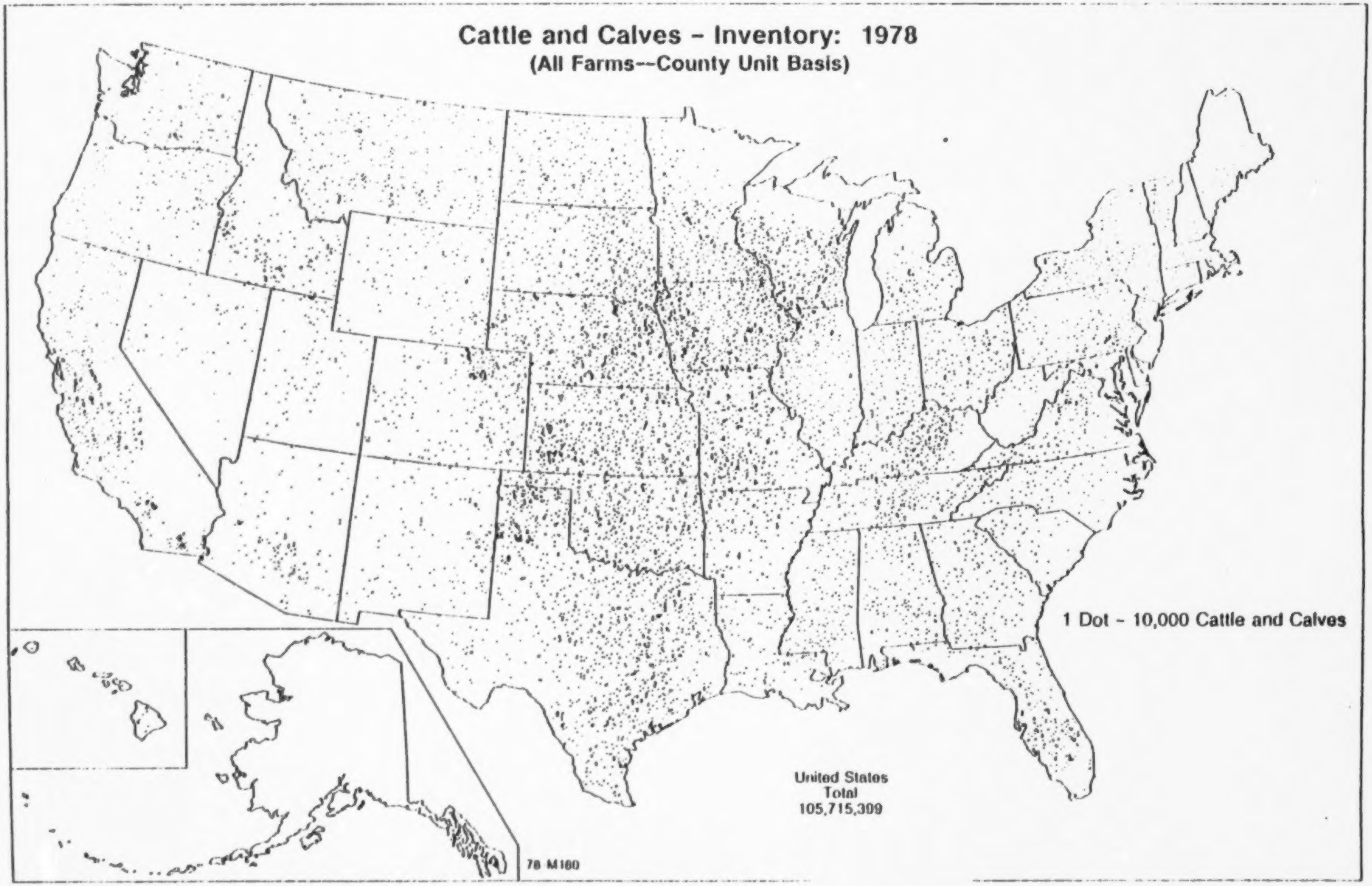
may be used in these applications, but they are too numerous to list here.

The use of the pathway identification approach depends on knowledge of the location of food generation areas and food storage, processing, and preparation areas. While the location of releases may not be known, knowledge of the distribution of food generation areas is useful in determining the probability of chemical contact with food. The location of food generation areas is largely discussed in the Census of Agriculture (USDOC 1981). This multi-volume report compiles extensive statistics on the number of livestock or acres of crop production by county for the entire U.S. Figure 6 shows an example of a graphic summary of some of these data. While cattle and calves and dairy cows, for example, are widely distributed, growing areas for some crops are very limited. The food grown in a given area can be determined roughly by using the maps in the graphic summary, or more specifically by using the county summaries for each state. Livestock and poultry are reported as number per county. Crops are reported by acres per county in the state summaries. More recently, these data have been converted to a more usable form for risk assessment. Two data bases exist that contain agricultural production on a county or lat/long basis. The livestock data are very useful in this data base, but the crop data are combined into groups which may or may not be useful for a particular assessment. (For access information see Section 3.2.3, Baes et al. 1985).

The Census of Agriculture (USDOC 1981) gives information on the location and production of fish farms, but not of commercial or sport fishing areas. The National Marine Fisheries Service (NMFS) of NOAA publishes various fishery statistics. NMFS (1980a) contains the most recent compilation of commercial fisheries statistics (1976). In addition, however, they publish annually "Fisheries of the United States" (NMFS 1983). This volume summarizes U.S. commercial landings by state and at about 120 major U.S. ports in pounds and dollars as shown in Tables 19 and 20. Marine recreational fishing is also summarized by the same agency in the "Marine Recreational Fishery Statistics" (NMFS 1980b). These statistics also summarize fish caught by state and various other characteristics.

Fresh-water recreational fishing statistics are not as well documented. The available information is summarized independently by each state and would not be practically accessible for a national analysis.

These data are not always in ideal form for use in this methodology. At this point in the methodology, however, it is important only to identify whether fish/shellfish, for example, are in the vicinity of a source at some point in their life-cycle. The compilations referenced above will provide data adequate for this purpose, at least for commercially important species.


Cattle and Calves - Inventory: 1978
(All Farms--County Unit Basis)
1 Dot - 10,000 Cattle and Calves
United States
Total
105,715,309
78 M180

Source: USDOC (1982)

FIGURE 6 EXAMPLE OF GEOGRAPHICAL DISTRIBUTION OF FOOD PRODUCTION

TABLE 19 U.S. COMMERCIAL LANDINGS

U.S. COMMERCIAL LANDINGS, BY STATES, 1981 AND 1982 (1)

State	1981		1982		Record landings	
	Thousand pounds	Thousand dollars	Thousand pounds	Thousand dollars	Year	Thousand pounds
Alabama.	33,677	44,148	27,362	47,348	1973	39,749
Alaska	975,245	639,797	878,935	575,569	1980	1,053,896
Arkansas	19,060	6,306	18,844	7,390	-	(2)
California	775,171	275,196	695,428	241,188	1936	1,760,183
Connecticut.	1,272	2,128	5,526	9,613	1930	88,012
Delaware	3,030	1,662	3,577	2,267	1953	367,500
Florida.	215,281	172,726	195,060	168,008	1938	241,443
Georgia.	18,589	13,158	20,075	22,344	1927	47,607
Hawaii	13,306	18,338	14,245	14,426	1954	20,610
Idaho.	496	28	496	26	-	(2)
Illinois	4,453	994	5,925	1,410	-	(2)
Indiana.	185	129	112	53	-	(2)
Iowa	3,741	945	4,826	1,266	-	(2)
Kansas	170	41	219	55	-	(2)
Louisiana.	1,168,597	193,549	1,718,668	230,383	1982	1,718,668
Maine.	238,107	103,945	217,379	100,900	1950	356,266
Maryland	115,115	56,640	100,478	51,438	1890	141,607
Massachusetts.	369,640	196,854	343,955	204,223	1948	649,696
Michigan	12,823	5,547	11,895	8,118	1930	35,580
Minnesota.	8,236	1,960	11,146	2,531	-	(2)
Mississippi.	264,891	30,159	383,767	39,877	1971	400,576
Missouri	970	231	1,251	310	-	(2)
Nebraska	111	29	143	39	-	(2)
New Hampshire.	7,690	4,162	7,586	3,776	-	(2)
New Jersey	188,396	48,283	90,190	45,007	1956	540,050
New York	36,522	45,555	35,778	45,392	1880	335,000
North Carolina	432,006	57,520	307,968	63,824	1981	432,006
North Dakota	727	117	938	157	-	(2)
Ohio	7,577	2.198	5,957	2,674	1936	31,033
Oregon	134,626	52,461	127,625	57,493	1978	134,557
Pennsylvania	343	189	108	79	-	(2)
Rhode Island	80,288	48,761	112,898	55,401	1889	128,056
South Carolina	16,232	14,161	19,902	23,731	1965	26,611
South Dakota	2,359	357	2,914	473	-	(2)
Texas.	113,108	174,787	89,219	165,197	1950	237,684
Virginia	487,919	69,124	690,677	68,768	1982	690,677
Washington	184,593	95,995	170,160	90,071	1941	197,253
West Virginia.	31	16	40	21	-	(2)
Wisconsin.	38,231	5,502	31,356	3,129	-	(2)
Other.	4,265	3,961	14,583	5,106	-	(2)
Total	5,977,069	2,387,739	6,367,310	2,389,093	1980	6,482,354

(1) Landings are reported in round (live) weight for all items except univalve and bivalve mollusks, such as clams, oysters, and scallops, which are reported in weight of meats (excluding the shell).

(2) Not determined.

Note:--Data are preliminary. Data do not include landings by U.S.-flag vessels at Puerto Rico and other ports outside the 50 States, or catches by U.S.-flag vessels unloaded onto foreign vessels within the U.S. FCZ (joint venture). Therefore, they will not agree with "U.S. Commercial Landings" table on page 8. Data do not include aquaculture products, except oysters and clams.

Source: NMFS (1983)

TABLE 20 U.S. COMMERCIAL LANDINGS

COMMERICAL FISHERY LANDINGS AND VALUE AT MAJOR U.S. PORTS, 1979-82

Port	Quantity 1979	1980	1981	1982
	Million pounds			
Cameron, La.	593.1	479.8	447.6	711.7
Los Angeles Area, Calif. (1)	373.2	330.1	373.6	331.8
Pascagoula-Moss Point, Miss.	293.3	291.9	220.5	331.0
Empire-Venice, La.	278.0	275.4	221.5	267.3
Dulac-Chauvin, La.	246.0	265.3	203.9	265.6
Gloucester, Mass.	160.2	210.0	166.0	144.3
Beaufort-Morehead City, N.C.	218.5	171.5	177.0	116.4
San Diego, Calif.	156.6	190.1	149.7	106.8
Kodiak, Alaska	160.5	207.4	193.2	105.3
New Bedford, Mass.	86.0	99.6	76.2	82.3
Portland, Maine	59.6	54.9	39.9	66.6
Rockland, Maine	41.8	56.0	41.7	57.2
Point Judith, R.I.	54.3	42.9	41.7	55.7
Dutch Harbor-Unalaska, Alaska	136.8	136.5	73.0	47.0
Newport, Oreg.	36.0	36.4	46.7	46.7
Astoria, Oreg.	40.4	39.8	44.8	45.0
Cape May-Wildwood, N.J.	58.3	51.5	42.7	44.9
Monterey, Calif.	(2)	(2)	49.8	44.5
Seattle, Wash.	16.5	10.0	25.0	44.4
San Francisco Area, Calif.	(2)	(2)	35.7	43.5
Petersburg, Alaska	31.3	32.3	30.0	38.8
Coos Bay-Charleston, Oreg.	23.5	27.0	36.5	37.0
Port Hueneme, Oxnard, and Ventura, Calif.	(2)	(2)	48.1	36.4
Eureka, Calif.	32.1	34.5	35.0	36.0
Akutan, Alaska	38.2	58.9	40.6	33.4
Hampton Roads Area, Va. (3)	27.2	23.8	29.1	33.2
Wanchese-Stumpy Point, N.C.	34.6	39.5	39.0	32.5
Boston, Mass.	30.3	34.4	28.1	27.2
Bellingham, Wash.	40.0	40.0	27.0	26.6
Ocean City, Md.	13.4	22.3	23.4	22.4
Westport, Wash.	25.0	23.0	24.0	21.1
Atlantic City, N.J.	(2)	(2)	18.1	19.9
Brownsville-Port Isabel, Tex.	22.0	21.5	28.9	19.0
Aransas Pass-Rockport, Tex.	19.0	22.1	24.4	18.0
Bayou La Batre, Ala.	21.8	19.9	25.1	17.8
Crescent City, Calif.	(2)	(2)	15.2	17.7
Fort Bragg, Calif.	(2)	(2)	15.7	16.3
Golden Meadow-Leeville, La.	15.6	15.4	18.5	14.2
Oriental-Vandemere, N.C.	19.5	19.8	17.1	14.0
Cape Canaveral, Fla.	(2)	(2)	17.0	12.5
Lafitte-Barataria, La.	10.4	11.1	14.7	11.9
Anacortes, Wash.	(2)	(2)	9.5	11.9
Santa Barbara, Calif.	(2)	(2)	14.1	11.0
Delacroix-Yscloskey, La.	(2)	(2)	(2)	10.6
Point Pleasant, N.J.	12.8	11.1	10.9	10.5
Delcambre, La.	(2)	8.6	11.0	10.4
Blaine, Wash.	10.5	10.0	8.1	10.1
Key West, Fla.	16.5	15.4	19.0	10.0
* Ilwaco, Wash.	(2)	(2)	16.8	9.9
Everett, Wash.	(2)	(2)	(2)	9.5
Fort Myers, Fla.	15.9	13.5	15.0	9.2
Freeport, Tex.	8.0	10.1	14.9	9.0
Apalachicola, Fla.	10.4	11.6	12.0	8.0
Brookings, Oreg.	9.8	9.5	7.6	7.7
Chincoteague, Va.	12.3	15.9	9.0	7.1
Darien-Bellville, Ga.	9.0	9.2	6.2	7.1
Galveston, Tex.	(2)	(2)	8.1	7.0
Cape Charles Oyster, Va.	9.7	8.1	7.5	6.5
Bon Secour-Gulf Shores, Ala.	(2)	(2)	7.0	5.9
Grand Isle, La.	(2)	(2)	7.1	5.6

Port	Value 1979	1980	1981	1982
	Million dollars			
Los Angeles Area, Calif. (1)	89.3	121.9	110.5	92.9
Kodiak, Alaska	73.4	84.5	*132.0	90.1
New Bedford, Mass.	67.4	71.3	77.9	54.6
San Diego, Calif.	62.7	110.6	93.0	53.7
Brownsville-Port Isabel, Tex.	50.0	42.2	43.4	52.0
Dulac-Chauvin, La.	41.5	50.0	51.5	51.7
Dutch Harbor-Unalaska, Alaska	92.7	91.3	57.6	47.8
Gloucester, Mass.	29.7	34.7	45.1	44.5
Aransas Pass-Rockport, Tex.	40.0	40.2	41.0	41.0
Cameron, La.	34.3	33.3	29.9	40.4
Empire-Venice, La.	28.8	31.0	30.5	36.4
Bayou La Batre, Ala.	34.9	23.7	31.4	33.8
Freeport, Tex.	25.0	19.9	26.8	26.0
Lafitte-Barataria, La.	16.6	14.8	20.8	21.9
Golden Meadow-Leeville, La.	22.5	12.2	19.9	21.5
Beaufort-Morehead City, N.C.	22.7	22.5	17.2	20.0
Point Judith, R.I.	11.0	11.5	13.2	19.9
Petersburg, Alaska	23.7	17.0	22.0	19.5
Key West, Fla.	25.9	18.3	27.0	19.0
Pascagoula-Moss Point, Miss.	18.1	18.5	16.8	18.5
San Francisco Area, Calif.	(2)	(2)	18.0	18.3
Cape May-Wildwood, N.J.	32.2	26.9	20.5	18.1
Delcambre, La.	14.8	13.3	18.8	17.6
Hampton Roads Area, Va. (3)	31.1	27.5	22.8	17.5
Bellingham, Wash.	18.3	15.2	12.0	16.9
Astoria, Oreg.	19.2	13.7	15.0	15.7
Seattle, Wash.	6.6	6.0	15.0	15.6
Akutan, Alaska	28.2	42.8	29.2	15.6
Galveston, Tex.	(2)	(2)	13.3	15.0
Newport, Oreg.	12.6	13.7	14.0	14.5
Coos Bay-Charleston, Oreg.	8.2	13.5	19.2	14.3
Portland, Maine	10.1	13.6	17.0	13.7
Wanchese-Stumpy Point, N.C.	13.0	13.0	12.7	13.0
Cape Canaveral, Fla.	(2)	(2)	15.9	12.8
Eureka, Calif.	14.3	11.0	13.5	12.4
Bon Secour-Gulf Shores, Ala.	16.0	7.7	11.6	12.4
Fort Myers, Fla.	17.9	10.9	18.0	11.9
Boston, Mass.	10.7	12.3	12.4	11.8
Rockland, Maine	(2)	8.4	13.4	11.1
Apalachicola, Fla.	10.1	11.3	12.3	10.2
Port Arthur-Sabine, Tex.	(2)	(2)	8.2	10.0
Ocean City, Md.	8.2	9.9	10.5	9.9
Crescent City, Calif.	(2)	(2)	8.2	9.8
Delacroix-Yscloskey, La.	(2)	(2)	(2)	9.8
Monterey, Calif.	(2)	(2)	10.4	9.3
Palacios, Tex.	(2)	(2)	(2)	9.0
Atlantic City, N.J.	(2)	(2)	7.9	8.8
Westport, Wash.	10.6	11.6	10.0	8.5
Anacortes, Wash.	6.1	5.4	7.2	8.0
Darien-Bellville, Ga.	8.7	7.5	4.6	7.9
Oriental-Vandemere, N.C.	6.6	9.1	6.5	7.7
Fort Bragg, Calif.	(2)	(2)	6.3	6.4
Port Lavacca, Tex.	(2)	(2)	(2)	6.0
Blaine, Wash.	(2)	4.0	3.6	5.7
Grand Isle, La.	(2)	(2)	7.8	5.7
Santa Barbara, Calif.	(2)	(2)	5.9	4.9
Brookings, Oreg.	(2)	3.8	3.8	4.6
Point Pleasant, N.J.	6.8	5.0	4.7	4.6
Chincoteague, Va.	6.5	8.0	5.1	3.9
Port Hueneme, Oxnard, and Ventura, Calif.	(2)	(2)	4.6	3.8

(1) Previously called San Pedro, Calif. (2) Not available. (3) Previously called Hampton-Norfolk, Va.

*Record. Record quantity was 848.2 million lb landed in San Pedro, Calif., in 1960.

Note.--Data for some ports are estimated. To avoid disclosure of private enterprise, the following ports were not included: Fernandina Beach, Fla.; Intercoastal City and Morgan City, La.; Chatham and Sandwich, Mass.; Biloxi, Miss.; Fort Monmouth-Belford, N.J.; Southport-Calabash, N.C.; Newport, R.I.; and Reedville, Va.

Source: NMFS (1983)

The potential for contact with water supplies used as drinking water for livestock and poultry and as irrigation water for crops can be identified to some extent by using a data base kept by the Office of Drinking Water, the Federal Reporting Data System--Public Water Systems. This data base documents public water supplies by county or city, giving source information, the population served, and the type of use. For access information, see Section 3.2.3.

The location of food storage and processing plants can be used to determine if products in storage or processing may become contaminated. The Chilton Company (1981) publishes annually a "Directory of U.S. Food and Beverage Plants." This compilation lists all food and beverage plants within a given county, along with the products produced and the peak employment. While this source provides the locations and products, it does not give volumes of production. Trinet, Inc. publishes share-of-market data (in percent sales) for each plant within a given SIC category. This information would provide an indication of the magnitude of production at a given facility which could later be used in estimating exposure. For access information see Section 3.2.3. The Census of Manufacturers (USDOC 1980) can provide the total volume of shipments for the U.S. within a SIC code. Thus, if desired, the volume of food shipped from a particular plant can be estimated.

Food preparation areas can include homes, restaurants, etc. so that almost any use that may result in releases to air or water has the potential for food contamination via this pathway.

A.3.4 Identification of Most Significant Contamination Pathways (Step 4)

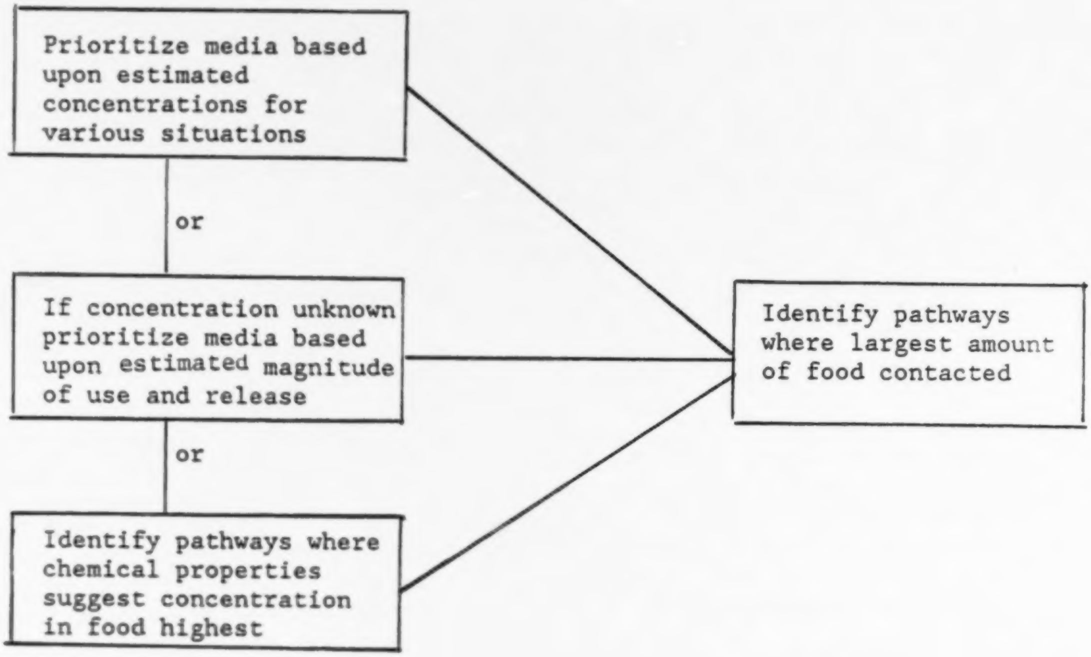
The relevant contamination pathways have been identified in Steps 2 and 3. This merely implies that given the nature of the chemical and its particular uses and releases, contact with food via a particular pathway may occur. While some pathways have been eliminated in this process, it is obvious that some of the remaining pathways are more significant than others. This section will address methods of assessing the significance of the relevant pathways using two criteria, the physical/chemical properties of the compound, and the amount of food potentially contaminated. Figure 7 summarizes the three factors which must be considered in this step.

1. The media contacting food can be prioritized by concentration of the chemical in the media (either quantitatively or qualitatively) for indirect pathways.

2. The relevant pathways can be prioritized using the physical/chemical properties of the compound and the pathway characteristics. The properties, as discussed below, are intended to provide a surrogate measure of concentrations in food.

FIGURE 7

PRIORITIZATION OF RELEVANT CONTAMINATION PATHWAYS


Prioritize media based upon estimated concentrations for various situations
or
If concentration unknown prioritize media based upon estimated magnitude of use and release
or
Identify pathways where chemical properties suggest concentration in food highest
Identify pathways where largest amount of food contacted

3. At the same time, the amount of food potentially contaminated must be considered.

The estimation of concentrations in environmental media is considered in Freed et al. (1985). The consideration of use and release characteristics in lieu of estimated concentrations is addressed below, as are the remaining two factors.

A.3.4.1 Prioritization of Relevant Pathways Based Upon Chemical Properties and Pathway Characteristics

This section presents a simple scheme that can be used to prioritize various food contamination pathways based upon the concentration of the toxicant expected in the contaminated food. The scheme requires consideration of the following:

(1) The amount of the chemical released;
(2) The chemical's persistence in the compartment(s) traversed;
(3) The chemical's rate of movement along a pathway;
(4) The chemical's mobility from the environmental compartment to food; and
(5) The number of steps in the pathway.

A simple scoring system is used since more sophisticated approaches (e.g., modeling) are not warranted due to their complexity and the unavailability of input data. The implementation of this scheme will require some subjective judgements. If this is done in a reasonable manner, the scheme should allow the user to identify pathways that are clearly more important than others. Small differences in scores for different pathways are not significant.

Some of the elements to be considered in this scheme (items 1-5 in the list above) may have already been considered in the initial selection of pathways. This may need to be taken into account in the implementation of this scheme. The next subsection of this report (A.3.4.2) will provide the prioritization scheme that will be based upon an assessment of the amount of food potentially contaminated.

Table 21 provides a summary list of the elements of the prioritization scheme. Each of the five items to be considered is listed along with a series of scores (1-3 or 0-3) to be assigned based upon the user's assessment of the item. It is suggested that when two or more pathways are to be scored (and the results compared), they should be scored by the same person. If no information is available on a particular item, or if it does not appear pertinent, then a mid-level score of 2 may be assigned.

After considering each of the five items, a summary score is obtained for each pathway by simple addition of the individual scores. These summary scores may then be used to identify high priority pathways. The maximum possible score is 15; the lowest, 4. Any chemical with a score of 3 on item 4 (i.e., there is some form of

TABLE 21 PRIORITIZATION SCHEME FOR RELEVANT PATHWAYS[a]

1. Amount Released to Compartment

Amount	Score
• Large ($> 10^3$ kg/yr)	3
• Moderate ($10 - 10^3$ kg/yr)	2
• Small (< 10 kg/yr)	1

2. Persistence in Compartment

Mean Lifetime	Score
• Long (>1 year)	3
• Moderate (1 week - 1 yr)	2
• Short (< 1 week)	1

3. Rate of Movement Along Pathway

Rate	Score
• Fast	3
• Moderate	2
• Slow	1

4. Mobility from Compartment to Food

Mobility (or Partition Coefficient)	Score
• High	3
• Moderate	2
• Low	1

5. Number of Steps in Pathway

No. Steps	Score
• Direct Contamination of Food Storage processing or preparation area	3
• 1 Step	2
• 2 Steps	1
• 3 or more Steps	0

[a] For guidance in scoring, see text

direct food contamination possible) should be given added priority in the final evaluation of pathways.

Each of the five criteria for scoring are briefly discussed below.

1) Amount Released to the Initial Compartment - To a first approximation, it can be assumed that the eventual concentration of the pollutant in food will be directly proportional to the amount released to a given compartment. For purposes of scoring, however, it may be easier to consider the logarithmic scale implied in Table 21 (10 kg/yr; 10 - 10^3 kg/yr; and 10^3 kg/yr). As long as different pathways are scored by the same criteria, the exact nature (linear vs logarithmic) should not be crucial.

2) Persistence in Compartment - The user should also consider the potential for degradation, by all reasonable mechanisms, within each compartment of each pathway. Degradation mechanisms may include, for example, biodegradation, hydrolysis, oxidation, and photolysis. While it is unlikely that appropriate rate constants for each of these reaction types will be available, it should be possible to assign a score to a chemical/compartment scenario based upon analogy with other known systems. If the persistence is deemed to be so significant that the mean lifetime of the chemical in the compartment (excluding considerations of bulk transport) would be longer than one year, a score of 3 is given. A mean life of 1 week - 1 year is scored 2; a mean life of less than 1 week is scored 1. A score of 0 might be appropriate for some chemicals with a mean life less than 1 day; such chemicals, unless involved in some direct food contamination incident, are unlikely to pose a problem.

3) Rate of Movement Along Pathway - Within a compartment or pathway, chemicals may have a wide range of mobilities due to both chemical and environmental properties. Just which properties will predominate will depend on the specifics of the food contamination pathway. In some cases, for example, bulk transport (with flowing water, air or sediment) may cause the chemical to be quite mobile and, thus, capable of reaching and contaminating the food item. On the other hand, transport out of the compartment may decrease mobility along the food contamination pathway. For example, volatilization from surface soils could reduce availability for plant uptake. In some cases, the mobility (or lack of it) will be tied primarily to chemical properties. For example, a chemical with a very high soil adsorption coefficient will not be very mobile in the unsaturated soil zone. Scoring for mobility in soil-groundwater systems using K_{oc} might be as follows: A compound with K_{oc} less than 100 might be scored as 3, 100-10,000 as a 2, and greater than 10,000 as a 1. In scoring, the food contamination pathway must be considered for the properties and/or bulk transport mechanisms that are relevant and how they may affect the chemical's movement along the pathway. Where a pathway actually consists of two or more distinct subpathways (which

must be traversed in series), the mobility in each subpathway/compartment should be assessed and a score (1-3) assigned based upon the slowest pathway.

4) Mobility from Compartment to Food - The ease with which the chemical can actually be taken up by plants and animals (food sources) is considered as a separate scoring item. No clear rules, based on species type and chemical properties, can be given that will allow a prediction of mobility in all cases. As noted in Section B.4 of this report, however, ease of uptake in plants is often strongly correlated with water solubility, even for cases where - as in foliar uptake - the uptake is not directly from water. The correlation of uptake in aquatic and terrestrial organisms with the octanol-water partition coefficient is described in Sections B.2.1 and B.3. Other factors which may be considered in assigning a score for this criterion are the probable differences in ease and rate of uptake via different routes, e.g. ingestion, inhalation, gill transport, skin absorption for animals, and root, stem, and foliar uptake by plants. As an example, scoring for fish bioaccumulation might be as follows: A compound with a BCF of less than 100 might be scored a 1, 100-1000 as a 2, and greater than 1000 as a 3.

5) Number of Pathway Steps - If direct contamination of food in food storage, food processing and/or food preparation areas is involved, a score of 3 is assigned. Lower scores (cf. Table 21) are assigned for pathways that are less direct and involve one, two or three (or more) steps. This criterion may involve some redundancy with the first four criteria. If so, the scoring here may be eliminated. However, the general concept here is that the more complex the overall pollutant transport pathway is, the more dilution and/or degradation there will be prior to possible food contamination. It appears reasonable to assign a very low priority to any pathway involving three or more subpathways (in series) unless the scores on the other criteria are all high.

The scorings suggested above are somewhat arbitary and may need to be revised based upon experience with the prioritization scheme. The important factors in scoring the mobility from compartment to food will also become evident with further use of the methodology.

A.3.2 Prioritization of Relevant Pathways Based Upon the Amount of Food Potentially Contaminated

The methodology described above, although somewhat subjective, allows the identification of pathways of contamination that are relevant for a given chemical and its uses and potential releases. In some situations the location of releases, the resultant concentrations, and the area of impact will be quantified. In these situations it would be possible to examine the amount of food potentially contaminated by various pathways. In many situations, however, the location will not be known specifically, but may be known generically. For example, a compound used as an adhesive may be released during production, the locations of which would probably be known. If this chemical were used in the manufacture of tires, the locations of releases from use would probably not be specifically known, and releases from tires themselves would be widely dispersed. In this example, concentrations would be expected to be greatest in both water and air around the production facilities. Use in tire manufacture would be expected to be more widely dispersed, resulting in lower environmental concentrations. The area impacted would be greater, however. Releases from tires would be widely dispersed and could be expected to result in relatively low concentrations in any medium and thus can probably be discounted as an important starting point for contamination pathways.

Where production locations are known, the examination of data sources can allow one to document the food items grown in the area, the water supplies used for drinking water for livestock or irrigation, and the food processing facilities located in the area. Many of these data sources are indexed by county. Two examples of such information are shown in Table 22. This table shows that a wide variety of products are grown even in areas that are not considered agricultural. If a production facility were to be located in Montgomery Co., OH, emissions to air and water would be considered for pathways resulting in contamination of meat and field crops. In comparison, meat and orchard fruit would be important considerations in Worcester Co., MA. The identification of food processing plants in these two counties is shown in Table 23. These data suggest that a variety of food products can be produced in a given county, although bread and dairy products appear to be common, at least in these two counties. Not surprisingly, corn syrup and other corn by-products are produced in Montgomery Co., OH. Also of interest is that soft drink bottling plants are found in both counties. Therefore, releases which may contaminate water supplies for these facilities would be of particular interest.

At this point in the methodology it is difficult to provide guidelines for prioritizing pathways by the amount of food potentially contaminated for several reasons:

- Some situations of release or contact are geographically defined, but many are not.

- For those situations that are geographically defined, Tables 22 and 23 show that collected information is in a wide variety of forms, and is not strictly comparable. To prepare such a table so that the units are consistent, for example, pounds of edible product present, would be extremely time-consuming and may not always be warranted.

- For those situations that are not easily geographically defined, for example, the use of an adhesive in tire manufacture,

TABLE 22
FOOD GENERATION IN TWO COUNTIES

	MONTGOMERY CO., OH	WORCESTER CO., MA
Food generated		
Meat		
cattle and calves	19,381 head	23,918 head
hogs and pigs	19,763 head	13,368 head
sheep and lambs	3,781 head	1,317 head
poultry		
laying	41,499	589,116
broilers	351	220
Fish/Shellfish		
commercial	probably none	probably none
sport	limited	limited
Plants		
Field Crops		
field corn (total)	36,282 acres	7,802 acres
field corn for grain	34,471 acres (2,819,796 bushels harvested)	453 acres (35,380 bushels harvested)
sorghum	97 acres	43 acres
wheat for grain	14,091 acres (534,065 bushels harvested)	0
soybeans for beans	36,562 acres (1,209,695 bushels harvested)	0
hay (excluding sorghum hay)	8,617 acres (17,976 tons dry)	29,234 acres (59,204 tons dry)
Vegetables		
irish potatoes	5 acres (287 cwt harvested)	53 acres (13,712 cwt harvested)
vegetables, sweet corn, melons	522 acres	1,316 acres
berries	84 acres	81 acres
land in orchards	499 acres	3,838 acres

Source: USDOC (1981)

TABLE 23

FOOD AND BEVERAGE PLANTS IN TWO COUNTIES

PLANT	Major Product
Ohio - Montgomery Co.	
Bluebird Baking Co., Dayton	Bread, cakes, pies
Borden, Inc., Dayton	Milk, cottage cheese, butter
Car-Mi Inc., Dayton	Corn syrup
Cargill Inc., Dayton	Corn syrup, corn starch, other corn by-products
Coca-Cola Bottling Co., Dayton	Soft drinks
Esther-Price-Candies, Inc., Dayton	Chocolate confections
ITT Continental Baking Co., - Wonder Bread Div., Dayton	Bread
Liberal Markets Inc., Concord Provision Co. Div., Dayton	Processed beef
Mikesell Daniel W. Inc. - Mike Sells Potato Chip Co., Dayton	Chips, snacks, popcorn
Milking Marketing Inc., Dayton	Canned milk products
Monsanto Co., Miamiburg	Hdqts.
National Industries Inc. - Hawthron Mellody Inc., Dayton	Milk
Pepsico Inc. - Holiday General Corp., Dayton	Soft drinks
Siegler Bottling Co., Inc., Dayton	Soft drinks
Superior Beef Inc., Dayton	beef (made in same estab. as basic materials) meat sauces, chocolate and cocoa extracts
United Belton, Inc., Dayton	Flavoring, extracts
MA - Worcester Co.	
Acme Boneless Beef Co., Inc. - Wilkinsonville	Processed beef--made from purchased material or mat. transferred from another establishment
American Potato Co., Roger Bros. Co.- Lunenburg	Processed pork--made from purchased material or mat. transferred from another establishment
Automatic Rolls of New England, Auburn	Bakery products
Deary Bros. Inc., Webster	Milk
Family Bakery Co., Inc., Worcester	Bakery products
Hillcrest Dairy, Inc., Auburn	Dairy products
Home of the Herbert Candies, Shrewsbury	Candy

TABLE 23 CONTINUED

FOOD AND BEVERAGE PLANTS IN TWO COUNTIES

PLANT	Major Product
MA - Worcester, Co.	
Larpson MH & Co., Inc., Worcester	Milk
Leroux Meats Inc., Holden	Sausage & Similar Prod.--made from purchased material or material transferred from another establishment
Lundgren & Jonaitis Dairy, Shrewsbury	Milk
Miles BF & Co., Millbury	Fresh Packed Vegetables & Juices
Millbrook Inc. Worcester	Fresh Packed Vegetables & Juices
Mt. Wachusett Dairy Inc., W. Boylston	Milk
Near East Food Products Inc., Leominster	Other Food Prep.
Nissen John J. Baking Co., Worcester	Bread and Rolls
Pepsi-Cola Bottling Co., Holden	Soft Drinks
Polar Corp. Worcester	Soft drinks
Portion Control Meat Pro., Wilkinsonville	Meat Packing Prod.--made in same estab. as basic materials
Snider Bros., Inc., Wilkinsonville	Prepared Meats--made from purchased material or materials transferred from another estab.
Squibb Corp. Dolbs-Life Savers, Worcester	Pies
Squibb Corp. Dolbs-Life Savers, Harvard	Bakery Products
Trappist Preserves, Spencer	Jams, jellies, preserves
Tri-Sum Potato Chip Co., Inc. Leominster	Chips, snacks, popcorn
United Crop Farmers Inc., Fitchburg	Poultry Feeds
Van Brode Milling Co., Clinton	Cereals, ready to serve

Source: Chilton Company (1981)

specific information on pathways cannot be developed by location. Prioritization in this case will depend on the chemical properties and the expected volume of release or resultant concentration in various situations.

As a result, prioritization of pathways will depend on the amount and type of information developed for a given chemical and will require judgement by the user in evaluating which pathways to consider for quantitative assessment. Depending on the scope of the assessment, it may be reasonable to identify the pathway that is likely to result in the highest concentration in food. This analysis can be carried through in order to determine whether food represents a significant exposure route to humans compared to other exposure routes. If food appears to be a significant exposure route, then further analysis of other contamination pathways is required.

A.4 ACCIDENTAL PATHWAYS OF CONTAMINATION

The previous section addressed the potential pathways of food contamination when a chemical is used as intended. However, there is a possibility of misuse or accidents. This section applies to chemicals not used as intended. The nature of these incidents is limitless and this methodology cannot detail all the possibilities, nor even suggest which ones are the most probable. This section will attempt to describe some common types of accidents. Using this information, scenarios for specific chemicals or products could be developed to evaluate the potential for food contamination in these situations.

It should be noted that knowledge regarding food contamination incidents is extremely limited (OTA 1979). Their detection is not common, and those that are detected generally involve widespread exposure problems, such as PCBs or methylmercury. Table 24 shows the reported food contamination incidents and the estimated cost associated with each incident. Most of the reported incidents involve pesticides, with the exception of PCBs, PBBs, and mercury. Some of these are probably isolated incidents and can be viewed as accidental in the context of this report. Problems associated with the more persistent compounds have involved normal use practices which resulted in contamination of the environment and resultant contamination of food.

Section A-2 divides the food preparation process into two major stages: food generation stages, and post-harvest stages. In this context, it is useful to divide the post-harvest stages into in-process stages and post-process stages. The following discussions will address common contamination problems in each of these three stages. Table 25 summarizes these accidental pathways.

A.4.1 Food Generation Stages

The food generation stages are probably the least controlled stages in the food process and almost all incidents described by the

TABLE 24 FOOD CONTAMINATION INCIDENTS

	Reported incidents	Total estimated Cost ($)
STATE		
Idaho	Dieldrin	$ 100,000
	PCP	3,000
Colorado	Dieldrin	100
	Mercury	3,700
Maryland	Mercury	23,000
Texas	Mercury	85,000
Indiana	Dieldrin	25,027
	Dieldrin	250,000
Michigan	Mercury	10,000,000
	PCB	30,000,000
	PCNB	100,000
	PBB	215,000,000
	Picloram	12,000
	Chlordane	2,500
	DDT	2,000
	Toxaphene	2,000
	Parathion	328
	Diazinon	13,700
	Pentachlorophenol	28,468
	PCB	150,000
	Dieldrin	12,500
		$255,813,323
FEDERAL		
USDA/FSQS	Pesticides	18,900,000
	Mercury	63,000
	PCB	7,450,000
	Phenol	350
		26,413,350
Total United States		$282,226,673

Source: OTA (1979)

TABLE 25 COMMON ACCIDENTAL FOOD CONTAMINATION PATHWAYS

Type of Contamination	Food Generation Stage	In-Process Stage	Post-Process Stage
Mislabeling	Pesticides, fertilizers animal health care product, feed additives	Food ingredients, sanitizers, building maintenance compounds, pesticides in storage and preparation areas, packaging materials	Food ingredients, pesticides, building maintenance compounds in warehouse or supermarket
Misuse	"	"	"
Cross-Contamination	Transporation vehicles	Backflow of sewage or other substances, dripback from stacks containers or surfaces	transportation vehicles
Spills	Contamination of aquatic organisms most common	not common	can occur on a small scale

OTA (1979) occurred in these stages. Accidents primarily seem to involve the purposeful addition of some product (pesticides, animal health care products, feed additives, etc.). Misapplication of these products is a common problem. Mislabeling is also common. While chemicals added to food in the generation stages are approved for this use, many of them also have other uses. Thus, the mislabeling of the same chemical intended for another use can occur. This may result in the food use of a formulation not intended for food. The presence of low level contaminants in these purposeful additions can also present a food contamination problem. This problem is compounded when mislabeling occurs, since the levels of impurities are likely to be higher in a non-food-grade chemical.

Spills occurring in the vicinity of food or feed generation areas, drinking water supplies for livestock and poultry, and irrigation water supplies can result in food contamination. Probably the most common occurrence of this type is a spill resulting in contamination of aquatic organisms.

Transportation represents another accidental pathway. Improper cleaning, or the carrying of unapproved substances in vehicles used for food can also result in contamination.

A.4.2 In-Process Stages

The in-process stages include steps from storage to packaging or preparation for consumer distribution. The nature of the accidents occurring at this stage is similar to those in the food generation stages. Mislabeling is still a problem, although this could include food ingredients as well as sanitizers, building maintenance compounds, and pesticides used in food storage areas. Misuse and improper storage of these chemicals can also result in food contamination. Backflow of sewage or other substances to process water can occur, as well as drip back from stacks.

Cross-contamination, or the use of improperly cleaned containers for other purposes can also be a problem. Similarly, the use of steam for blanching or cooking can result in food contamination problems in commercial operations, particularly if the steam is not intended for food, and boiler additives not approved for food have been used.

Packaging represents a point of contact with food, sometimes for extended periods. Mislabeling or misuse of chemicals in the packaging material or adhesives, can coatings, etc. can result in contamination of the food item.

A.4.3 Post-Process

Contamination of food in the post-process stage basically consists of contamination of consumer goods. Contamination can result from spills, transportation, and improper formulation, especially related to mislabeling. Food may be contaminated in warehouses where storage of items may occur, in grocery stores, or in the home. Contamination occurring at this stage would not be likely to result in exposure to a large number of people.

APPENDIX B QUANTITATIVE METHODS

B.1 INTRODUCTION AND SUMMARY

This section presents calculational approaches for assessing the potential of pollutant migration into food. These approaches have not been presented in the form of a step-by-step procedure or a model, because of the uncertainty governing pollutant migration related to food. The intent is to provide a basis for estimation and an understanding of the factors that influence food contamination.

Table 17 showed that there are four major categories of food that can be segregated in terms of having unique contamination pathways. In the food generation stages, pathways to meat, crops, and fish/shellfish will be considered. In the post-harvest stages, food is considered as a whole, as contamination pathways are more dependent on processing method than on food type. Chemical losses are also discussed in this section. The pathways of chemical losses are similar to those of contamination transfer in the post-harvest stages.

A summary of the quantitative methods described in this section is shown in Table 26. The equations and relationships shown are to be used with caution. Table 26 gives a reference to the section in which more detail is provided. Table 27 summarizes the important physical/chemical properties that are needed to quantify contamination from each pathway. Quantification methods for each of these pathways will be considered below.

B.2 PATHWAYS TO ANIMALS

There are several pathways that can result in pollutant contamination of edible animal products in the environment as shown in Table 17. Among these contamination pathways to animals one might include:

- ingestion of feed grown in contaminated soil or from areas in which pollutant deposition has occurred on plants and/or soil,
- ingestion of drinking water originating from contaminated ground or surface water sources (from pollutant releases to soil or water) or from areas in which deposition has occurred (from pollutant releases to air),
- inhalation of pollutants released to air, and
- dermal absorption of vapors released to air or absorption of pollutants from contact with soil or contaminated water.

Residue levels found in edible animal tissues and products reflect the digestive and metabolic processes inherent in the species of concern, the time elapsed since exposure ceased, the biological half-life of the contaminant and its various metabolites that may appear as residues in food, the contaminant's lipid affinity or tissue binding, and its stability. The least desirable contaminant from a human health

TABLE 26 SUMMARY OF QUANTITATIVE METHODS

PATHWAYS	EQUATIONS	DEFINITIONS	COMMENTS	REFERENCE
PATHWAY TO ANIMALS (Section B.2)				
Ingestion of Contaminated Feed or Water				
	$C_T=(BF_f)(F)C_D$	C_T =conc. of chem. in tissue (ug/kg) BF_f=bioconcentration factor (fat basis) for organism of concern ((ug/kg fat)/(ug/kg of diet)) F =fat content of tissue (kg fat/kg tissue) C_D =concentration of pollutant in diet (or drinking water)(ug/kg)		
	Method 1 $\log BF_f=-1.476-0.495 \log S$	S =water solubility (ppm)	Regression using 23 chemicals, mainly chlorinated herbicides and pesticides, and wide ranges of values for independent variables.	Kenaga (1980)
	$=-3.457+0.500 \log K_{OW}$	K_{OW}=octanol-water partition coefficient		
	$=-3.825+0.701 \log K_{OC}$	K_{OC}=organic carbon water adsorption coefficient		
	$=-3.839+0.869 \log BCF_f$	BCF_f=bioconcentration factor in fish in flowing water tests	Criticized by Garten and Trabalka (1983) for use of questionable data. Confidence limits covered nearly 4 orders of magnitude.	
	$=-2.842+0.674 \log BCF_t$	BCF_t=bioconcentration factor in fish in static water terrestrial systems.		
	Method 2 $\log K_{OW} \leq 3.5$; no appreciable bioaccumulation in fat; i.e. $BF_f <$ 0.3 log S >4; No appreciable bioaccumulation in fat; i.e., BF_f <0.03	As above	Screening levels only. False positive/false negative error rate of 25% with 68 chemicals Not applicable to chemicals that can covalently bond or bind to proteins rather than fat.	Garten and Trabalka (1983)
Inhalation of Pollutants in Air				
	No Available Method			

TABLE 26 SUMMARY OF QUANTITATIVE METHODS (CONTINUED)

PATHWAYS	EQUATIONS	DEFINITIONS	COMMENTS	REFERENCE
Dermal Absorption				
	$F_s = K_s \Delta C$	F_s = flux or permeation rate through skin ($mg/cm^2 \cdot hr$) K_s = permeability constant ($l/cm^2 \cdot hr$) ΔC = concentration difference across skin (mg/l)	Fick's Law	Brown et al (1984)
	$K_{si} = K_{sj} (MW_j/MW_i)^{1/2}$	K_{si} = permeability constant of chemical i ($l/cm^2 \cdot hr$) K_{sj} = permeability constant of chemical j ($l/cm^2 \cdot hr$) MW_i = molecular weight of chemical i MW_j = molecular weight of chemical j		
PATHWAYS TO FISH/SHELLFISH (Section B.3)				
	$C_{ao}=(BCF)C_w$	BCF=bioconcentration factor in fish (ug/kg / ug/l) C_{ao}=concentration of pollutant in aquatic organism at equilibrium (ug/kg) C_w=concentration of pollutant in water (ug/l)		
	Method 1 Log BCF=0.76 log K_{ow}-0.23	K_{ow}=octanol-water partition coefficient	Regression with 84 chemicals and K_{ow} between 7.9to 8.1×10^6.	Bysshe (1982)
	=2.791-0.564 log S	S= water solubility (ppm)	Regression with 46 chemicals and S between 0.001 and 50,000 ppm.	
	=1.119 log K_{oc}-1.579	K_{oc}=soil (or sediment) adsorption coefficient	Regression with 13 chemicals and K_{oc} 1 to 1.2×10^6. Wide classes of chemicals represented by equations, but only a few fish species.	

TABLE 26 SUMMARY OF QUANTITATIVE METHODS (Continued)

PATHWAYS	EQUATIONS	DEFINITIONS	COMMENTS	REFERENCE
	Method 2 $BCF = 0.048\ K_{ow}$	as above	Used by EPA's TOX-SCREEN, screening level program.	Mackay (1982)
PATHWAYS TO CROPS (Section B.4)				
Uptake from Air				
	Method 1 $C_p = C_a RT/H$	C_p=concentration of pollutant in plant (ug/ml) C_a=concentration of pollutant in air (ug/mg) H=Henry's Law Constant (m^3 atm/mol) R=Gas Constant (8.2×10^{-5} m^3 atm/mol °K) T=Temperature (°K)	Theoretical, not tested with empirical experimental data.	
	Method 2 $C_p = \frac{r}{Y_v \lambda_{ei}} [1-(1-e^{-\lambda_{ei} t_e})/(\lambda_{ei} t_e)]$ x (deposition rate)	r = empirically determined initial reception fraction Y_v = vegetative productivity (g/m^2) λ_{ei}=empirical weathering constant (day^{-1}) t_e=crop growth period before harvest or grazing (days) deposition rate (g/m^2-day)	Equation derived from interception of radionuclides A number of empirical values required which are unknown for organic chemicals.	Chamberlain (1970)
Root Uptake				
	Method 1 $RCF = C_R/C_{es}$	RCF=root concentration factor C_R=concentration in roots (ug/ml) C_{es}=concentration in external solution (ug/ml)		Briggs et al (1982)

TABLE 26 SUMMARY OF QUANTITATIVE METHODS (Continued)

PATHWAYS	EQUATIONS	DEFINITIONS	COMMENTS	REFERENCE
	$TSCF=C_{ts}/C_{es}$	TSCF=transpiration stream concentration factor C_{ts}=concentration in transpiration stream (ug/ml) C_{es}=concentration in external solution (ug/ml)		Briggs et al. (1982)
	$\log(RCF-0.82)=0.77\log K_{ow}-1.52$ $TSCF=0.784\ \exp-((\log K_{ow}-1.78)^2/2.44))$ RCF= 0.82 (for polar species)	K_{ow}=octanol-water partition coefficient	Regression equations for 18 compounds (non-ionic O-methylcarbamoyloximes and substituted phenylureas) in barley shoots grown in nutrient solutions. Root physiology or rapid metabolism in roots may result in lower TSCF values than predicted.	Briggs et al. (1982)
	Method 2 $RCF_s=C_R/C_s$ $TSCF_s=C_{ts}/C_s$ $\log(RCF_s\ K_{oc}(OC)-0.82)=0.77\log K_{ow}-1.52$ $TSCF_s\ K_{oc}(OC)=0.784\ \exp-((\log K_{ow}-1.78)^2/2.44))$ $RCF_S\ K_{oc}(OC)=0.82$ (for polar species)	C_s=total concentration in soil (ug/cm^3) other definitions as above K_{oc}=soil adsorption coefficient OC=fractional organic carbon (g/g) Other definitions as above	As above	Derived from Briggs et al. (1982)
	Method 3 $C_{pl}=BC_{pl}\times C_o$ $K_d=K_{oc}(\%OC)$	C_{pl}=mature plant parts concentration (ug/g dry weight) BC_{pl}=bioconcentration factor in mature plant parts	Used by EPA's TOX-SCREEN, screening level program. Values of A and B used in TOX-SCREEN are 3.02 and -0.85	USEPA (1984b)

TABLE 26 SUMMARY OF QUANTITATIVE METHODS (Continued).

PATHWAYS	EQUATIONS	DEFINITIONS	COMMENTS	REFERENCE
	$\ln K_d = A + B \ln(BC_{pl})$ or $\ln(K_{oc}(\%OC)) = A + B\ln(BC_{pl})$	C_o=soil concentration (ug/g dry weight) K_d=soil-water partition coefficient K_{oc}=soil adsorption coefficient %OC=percent organic carbon A and B are empirically derived constants	respectively based on literature review of 21 elements.	
PATHWAYS TO FOOD-POST-HARVEST STAGES (Section B.5) Food in Contact with Air, Water or Liquid				
	DIFFUSION: $F = -D(dC/dx)$	F=pollutant mass flux along direction x ($ug/cm^2 \cdot sec$) D=diffusion coefficient of pollutant in food (cm^2/sec) C=concentration of pollutant in medium (ug/ml) dC/dx= concentration gradient in direction x (ug/ml·cm)	Fick's law	
	From Air to Food Air $F_1 = D_{fa}{}^*(C_a - C_{fa})/r$	F_1=pollutant mass flux across food surface ($ug/cm^2 \cdot sec$) $D_{fa}{}^*$=apparent diffusion coefficient of pollutant in food air (cm^2/sec) C_a=concentration of pollutant in air (ug/ml) C_{fa}=concentration of pollutant in food air (ug/ml) r=approx. radius of food particle (cm)	Many independent variables may have to be estimated. Additional equations for estimation of these parameters are shown in Appendix B or references provided.	

TABLE 26 SUMMARY OF QUANTITATIVE METHODS (Continued)

PATHWAYS	EQUATIONS	DEFINITIONS	COMMENTS	REFERENCE
	$D_{fa}^{*}=D_a(n_{air}^{10/3}/n_f^2)$ $n_{air}=n_f-m$	D_a=diffusion coefficient of pollutant in air (cm^2/sec) n_{air}=food-air filled porosity (ml/ml) n_f=food (total) porosity (ml/ml) m=food water content (ml/ml)		
	$\bar{F}_1=F_1/2$ for $C_{fa}=0, t=0$ sec $C_t=C_i+(\bar{F}_1 At)/M$	$\bar{F}_1$=average pollutant mass flux across surface (ug/cm^2·sec) C_t=concentration of pollutant in food after time t (ug/kg) C_i=initial pollutant concentration in food (ug/kg) t= time (sec) M=mass of food piece (kg) A=surface area of food piece (cm^2)	Estimates average concentration in food. Concentration varies spatially and with exposure time. Does not consider deposition of particulates.	
	From External Liquid to Food Liquid $F_2=D_{fm}^{*}(C_{el}-C_{fm})/r$	F_2=pollutant mass flux across food surface (ug/cm^2·sec) D_{fm}^{*}=apparent diffusion coefficient in food moisture (cm^2/sec) C_{el}=concentration of pollutant in external liquid (ug/ml) C_{fm}=concentration of pollutant in food moisture (ug/ml) r=approx. radius of food particle (cm)	Many independent variables may have to be estimated. Estimation methods provided in Appendix B or references provided.	
	Similar equations as diffusion from air to food air	Similar definitions as diffusion from air to food air	Estimates average concentration in food. Concentration varies spatially and with exposure time.	

TABLE 26 SUMMARY OF QUANTITATIVE METHODS (Continued)

PATHWAYS	EQUATIONS	DEFINITIONS	COMMENTS	REFERENCE
	PARTITIONING:			
	Moisture-Solid Partitioning $S=x/M=KC_{el}^{1/n}$	S=adsorbed concentration of contaminant on food particles (ug/g food) x=adsorbed pollutant mass on/in food (ug) M=mass of food (g) K=adsorption (partitioning) coefficient (ug/g)/(ug/ml) C_{el}=dissolved concentration of pollutant in external liquid (ug/ml) n=Freundlich isotherm parameter	quations adapted from similiar equations derived for organic soils and assumed valid for food. Assumes equilibrium.	
	$K=K_{ow}(\%lipid)/100$	K_{ow}=octanol-water partition coefficient		
	Moisture-Air Partitioning $C_{fa}=C_{fm}\ H/RT$	C_{fa}=concentration in food-air (ug/ml) C_{fm}=concentration in food-moisture (ug/ml) H=Henry's Law Constant (m^3 atm/mol) R=gas constant ($8.2x10^{-5}$ m^3 atm/mol °K) T=temperature (°K)	Derived from Henry's Law applicable to dilute solutions. Theoretical. Food solution is usually not dilute.	
Food in Contact with Surfaces	$M_t=2C_{op}(D_p t/\pi)^{1/2}$	M_t=amount migrated at time t (g/cm^2) C_{op}=initial chemical concentration in surface (g/cm^3) D_p=effective diffusion coefficient through surface (cm^2/sec)	For porous surfaces, e.g., soil, gives maximum amount of chemical that could migrate out.	Schwope et al. (1984)

TABLE 26 SUMMARY OF QUANTITATIVE METHODS (Continued)

PATHWAYS	EQUATIONS	DEFINITIONS	COMMENTS	REFERENCE
		t=time of contact of food with surface (sec)		
	$D_p = D_a(n_{air}^{10/3}/n_s^2)$	D_a=diffusion coefficient of pollutant in air (cm^2/sec) n_{air}=surface air-filled porosity (ml/ml) n_s=surface total porosity (ml/ml)		
	$C_f = 2C_{op}(D_p t/\pi)^{1/2} A_f/V_f$	C_f=average concentration of chemical in food (g/cm^3) A_f=surface area of food in contact with surface (cm^2) V_f=volume of food (cm^3)	Gives maximum average concentration in food. Concentrations would vary spatially.	
	Max. Conc. is limited by: $K = K_{ow}$ (% lipid)/100	K=adsorption (partitioning) coefficient (ug/g)/(ug/ml) K_{ow}=octanol-water partition coefficient	Assumes equilibrium.	
Additives				
	$C_f = C_i + \frac{C_a M_a}{M_f + M_a}$	C_f= final concentration of the pollutant in food (ug/kg) C_i=initial concentration of pollutant in food (ug/kg) C_a=concentration of pollutant in additive (ug/kg) M_a=mass of substance added (kg) M_f=mass of food to which substance was added (kg)	Concentration of substance in additive and mass of additive needs to be known.	
CHEMICAL LOSSES (Section B.6)				
	Similar to the equations for pathways to food-post-harvest stages.			

TABLE 27 IMPORTANT PHYSICAL/CHEMICAL PROPERTIES NEEDED FOR QUANTIFICATION OF EACH PATHWAY

Pathway	Section in Appendix	Physical/Chemical Property and Definition	Unit
PATHWAYS TO ANIMALS	B.2		
Ingestion of Feed or Water	B.2.1	S Water solubility, or	ppm
		K_{ow} Octanol-water partition coefficient, or	--
		K_{oc} Organic carbon soil adsorption coefficient, or	--
		BCF_f Bioconcentration factor in fish in flowing water tests, or	--
		BCF_t Bioconcentration factor in fish in static water systems	--
Inhalation of Pollutants Released to Air	B.2.2	No Available Method	
Dermal Absorption	B.2.3	K_s Permeability constant	$1/cm^2$ hr
PATHWAYS TO FISH/SHELLFISH	B.3	K_{ow} Octanol-water partition coefficient, or	--
		S Water solubility, or	ppm
		K_{oc} Soil (or sediment) adsorption coefficient	--
PATHWAYS TO CROPS	B.4		
Uptake from Air	B.4.1	H Henry's Law Constant	m^3atm/mol
Root Uptake	B.4.2	K_{ow} Octanol-water partition coefficient, or	--
		K_{oc} Soil adsorption coefficient	--

TABLE 27 IMPORTANT PHYSICAL/CHEMICAL PROPERTIES NEEDED FOR QUANTIFICATION OF EACH PATHWAY

Pathway	Section in Appendix	Physical/Chemical Property and Definition	Unit
PATHWAYS TO FOOD-POST-HARVEST	B.5		
Diffusion from Air to Food Air	B.5.1.1.1	D_a Diffusion coefficient of pollutant in air	cm^2/sec
Diffusion from External Liquid to Food Liquid	B.5.1.1.2	D_w Diffusion coefficient of pollutant in water	cm^2/sec
Moisture-Solid Partitioning	B.5.1.2.1	K Adsorption (partitioning) coefficient	(ug/g)/(ug/m
		K_{ow} Octanol-water partition coefficient	--
Moisture-Air Partitioning	B.5.1.2.2	H Henry's Law Constant	m^3 atm/mol
Food in Contact with Surfaces	B.5.2	D_a Diffusion coefficient in air	cm^2/sec
		K Adsorption (partitioning) coefficient, or	(ug/g)/(ug/m
		K_{ow} Octanol-water partition coefficient	
Additives	B.5.3	--	--
CHEMICAL LOSSES	B.6	As in Pathways to Food-Post-Harvest	

perspective is a toxic compound that is very stable or degrades to persistent and toxic residues in edible products.

B.2.1 Ingestion of Contaminated Feed or Water

Dairy cattle, beef cattle, swine, sheep, and poultry can all be inadvertently exposed to contaminated feed or water. This can occur from ingestion of contaminated water or plants and/or soil which contain pesticide residues or other pollutants, ingestion of plants capable of accumulating toxic materials from soil (e.g., selenium in cereal crops), or forage along highways or around industrial areas.

Use of municipal sludge as crop fertilizer and the practice of allowing food animals to graze on croplands after sewage sludge has been applied is another source of possible contamination. Municipal sludges typically contain heavy metals such as cadmium, chromium, nickel, copper, and lead as well as refractory organic compounds such as PCBs. Elevated levels of metals, particularly cadmium, have been found in sheep fed silage corn grown in municipal sludge-amended soil (Telford et al. 1982) and in steers fed a normal cattle ration plus 12% by weight of air-dried municipal sewage sludge (Boyer et al. 1981). The levels of lead and cadmium in kidneys, and of lead, cadium and copper in liver from these steers were high enough to cause toxicological concern for human consumption of these tissues.

Another point to keep in mind with respect to contamination of human food supplies is that ruminants may react to toxicants quite differently than non-ruminants due to differences in digestive structure and function between these two groups of animals. For example, ability to vomit effectively is different in ruminants and non-ruminants. Many monogastric animals (man, dog) vomit easily. Ruminants can vomit but the reflex is not as easily stimulated and the degree to which vomiting is effective in removing poisonous materials from the gut is much less in ruminants than in non-ruminants.

Determinations of human exposure to contaminants in edible animal tissues and products require information about the nature and amount of residues in the principal edible tissues (i.e., muscle, liver, kidney and fat; skin for poultry) and products (eggs, milk). Perhaps the most useful tool in this regard is data on the partition coefficients in octanol and water, which can be used as an indication of lipid affinity. A lipophilic tendency is a primary consideration in identifying compounds with long biological half-lives and thus potential animal residue problems for humans.

Theoretically, the concentration of a chemical in animal tissues may be estimated by:

$$C_T = (BF_f)\ (F)\ C_D \tag{B-1}$$

where C_T = concentration of chemical in tissue (ug/kg)
(BF_f) = bioconcentration factor (fat basis) for organism of concern (ug/kg of fat)/(ug/kg of diet)
F = fat content of tissue (kg fat/kg tissue)
C_D = concentration of pollutant in diet (or drinking water) (ug/kg)

Kenaga (1980) attempted to relate the bioconcentration factor of chemicals in terrestrial organisms with physical and chemical properties (water solubility, S; octanol-water partition coefficient, K_{ow}; organic carbon soil adsorption, K_{oc}); and bioconcentration factors in fish. Using 23 chemicals, the regression equations obtained for beef fat are shown in Table 28.

Garten and Trabalka (1983) criticized the regression equations derived by Kenaga (1980) for the use of questionable data for some independent variables. The bioaccumulation data for fish were derived from a variety of different methods, and data from unpublished reports were used. The confidence limits for Kenaga's predicted bioaccumulation factors covered nearly 4 orders of magnitude as shown in Table 28. Garten and Trabalka (1983) proposed screening levels as alternatives to estimation. A screening level was defined as the value of log K_{ow} below (or log S above) which no compound tested exhibited appreciable bioaccumulation in terrestrial organisms (birds, ruminants, non-ruminants). An arbitrary log BF_f of -0.5 was chosen as the limit which corresponded to 0.3 mg/kg in fat. The screening levels developed by Garten and Trabalka (1983) by this method are shown in Table 29. Garten and Trabalka (1983) also tested Kenaga's (1980) suggestion to use measured bioconcentration factors in aquatic test systems to predict bioaccumulation in terrestrial vertebrates. They found that bioconcentration in mammals and birds was very weakly correlated or uncorrelated with pollutant bioconcentration factors from fish studies (correlation factors 0.09-0.43), indicating that accurate prediction of bioaccumulation in birds or mammals cannot be obtained from fish tests alone. They did find, however, that bioaccumulation factors in sheep, poultry, rodents, dogs, cows and swine were significantly correlated and that bioaccumulation factors in rodents were highly correlated with bioaccumulation factors in poultry and cows.

The model TOX-SCREEN (USEPA 1984b) uses the screening method developed above by Garten and Trabalka, without attempting to quantify the actual level of bioaccumulation in terrestrial organisms.

B.2.2 Inhalation of Pollutants Released to Air

Livestock can potentially absorb pollutants via inhalation of vapors, respirable dust particles, or aerosols such as the spray drift from insecticide usage. Indeed, many agricultural processes involve actions which generate airborne dust. Unfortunately, there is an almost total lack of data regarding this route of animal exposure and there are no available methods to quantify resultant animal concentrations.

The types of information needed to adequately assess exposure of animals via this pathway and allow estimation of human exposure via food would include:

- the form of exposure - vapor or aerosol,
- if an aerosol, the particle size distribution,

TABLE 28 . BIOCONCENTRATION FACTORS OF CHEMICALS IN BEEF

Regression Equation	Equation No.	95% Confidence Limits	Correlation Coeff. = r
$\log BF_f = -1.476 - 0.495 \log S$	(B-2)	1.85	-0.817
$\log BF_f = -3.457 + 0.500 \log K_{ow}$	(B-3)	1.97	0.790
$\log BF_f = -3.825 + 0.701 \log K_{oc}$	(B-4)	2.19	0.732
$\log BF_f = -3.839 + 0.869 \log BCF_f$	(B-5)	2.05	0.771
$\log BF_f = -2.842 + 0.674 \log BCF_t$	(B-6)	1.58	0.879

Regression using 23 chemicals, mainly chlorinated herbicides and pesticides, where: S = water solubility, 0.002 - 502,000 ppm

K_{ow} = octanol-water partition coefficient, 0.02-1,400,000

K_{oc} = organic carbon soil adsorption coefficient, 2-468,000

BCF_f = bioconcentration factor in fish in flowing water tests, 0.6-61,600

BCF_t = bioconcentration factor in fish in static water terrestrial ecosystem tests, 0-84,500

BF_f = bioconcentration factor (fat basis), 0.0003-3.5 (ug/kg of fat)/(ug/kg of diet)

Source: Kenaga (1980)

TABLE 29 SCREENING LEVELS[a] FOR BIOCONCENTRATION IN BIRDS, RUMINANT AND NON-RUMINANT MAMMALS

Screening Level	Log BF_f	False positive/False negative Error Rate[b]
log $K_{ow} < 3.5$	No appreciable bioacc. in fat, log $BF_f < -0.5$ (or $BF_f < 0.3$)	25% with 68 different chemicals
log $S > 4$ (or $S > 10$ mg/l)	No appreciable biaocc. in fat, $BF_f < 0.03$ an order of magnitude less than screening levels	25% with 68 different chemicals

a. Value of log K_{ow} below or log S above which log $BF_f < -0.5$ (or 0.3 mg/kg in fat).

b. Particularly with respect to bioaccumulation of chemicals that can covalently bond or otherwise bind to proteins rather than fat (e.g., methylmercury).

Source: Garten and Trabalka (1983)

- the degree of absorption at the site of original contact,
- the rate and pattern of extracellular and intercellular distribution,
- metabolism, if any, at the absorbing and target tissues, and
- the rate of excretion and bioaccumulation.

The likelihood of having this information is small. However, some generalities can serve as guides for making estimates of exposure. Absorption of lipid-insoluble substances from the lung is a fairly rapid process, possibly more so than from the gastrointestinal tract. Lipid-soluble substances appear to be absorbed from the lungs even more rapidly, at rates that are presumably dependent on lipid/water partition coefficients. If exposure is to an aerosol or dust, knowledge of the particle size can help to define exposure. The filtering mechanisms of the respiratory tract are capable of excluding larger particles (diameter greater than 10 um) and only particles below 2 um actually reach the alveoli.

B.2.3 Dermal Absorption

Cutaneous penetration depends largely on the nature of the agent and is primarily a function of solubility and the rate of diffusion. The pH, extent of ionization, molecular size, temperature, humidity, and skin site also affect absorption through skin. In addition, the status of the exposed skin is important. Breaks in the skin, scratches, cuts, and scabs represent sites of easy entry for materials which might otherwise be excluded.

In general, lipid-soluble compounds as a group are better absorbed through skin than are water-soluble compounds. In the absence of skin-compound partition coefficients, solvent systems such as octanol-water or mineral oil-water partition coefficients can be used as models for estimating skin penetration of xenobiotic materials. It should be noted, however, that considerable variation exists among available solvent models and that no one system has been validated over a broad range of unrelated chemical structures. In addition, issues such as changing skin characteristics with abrasion, solvent exposure, or variations in the thickness of the stratum corneum are not approached in any of these solvent models.

To estimate the rate of diffusion of a pollutant from the surface of skin into the underlying tissue, Fick's law as expressed below may be used:

$$F_s = K_s \Delta C \qquad \text{(B-2)}$$

where: F_s = flux or permeation rate through the skin (mg/cm^2 - hr)
K_s = permeability constant (l/cm^2 - hr)
ΔC = concentration difference across the skin (mg/l)

C may be approximated to be equal to the concentration in the solution in contact with the skin of the animal. Brown et al. (1984) calculated permeability constants for ethylbenzene, styrene and toluene from experimental data for human skin at high concentrations. Data for permeability is not likely to be available for the chemical of concern. The values obtained by Brown et al. (1984) range from 0.0006 - 0.001 $1/cm^2$ - hr. K_s is directly related to the diffusivity of the chemical and may be estimated from:

$$K_{si} = K_{sj} (MW_j/MW_i)^{1/2} \quad \text{(B-3)}$$

where:
K_{si} = permeability constant of chemical i ($1/cm^2$ - hr)
K_{sj} = known permeability constant of chemical j ($1/cm^2$ - hr)
MW_i = molecular weight of chemical i
MW_j = molecular weight of chemical j

The method described above has not been tested and is based on very little information. The method is expected to provide very rough estimates of concentrations.

B.3 PATHWAYS TO FISH/SHELLFISH

Table 15 showed that the primary contamination route for aquatic species is absorption from water. While ingestion of contaminated food represents a possible contamination route, such a pathway would be difficult to quantify.

Pollutant concentrations in aquatic organisms are estimated using the concentration in water and a bioconcentration factor, BCF, for fish:

$$C_{ao} = (BCF)\, C_w/\rho_w \quad \text{(B-4)}$$

where
C_{ao} = concentration of pollutant in aquatic organism at equilibrium (ug/kg)
BCF = concentration of pollutant in aquatic organism/concentration in water
C_w = concentration of pollutant in water (ug/l)
ρ_w = density of water (kg/liter)

Bioconcentration factors have been measured for certain fish species under specific conditions. There are also several methods for estimating bioconcentration factors as described in Bysshe (1982). The methods recommended by Bysshe are summarized in Table 30. Before using the regression equations given, Bysshe (1982) and any recent review articles on actual measurements of the bioconcentration of the chemical of concern should be reviewed in case a measured value for bioconcentration is available. If measured values for independent variables are not available, estimation methods are available in Lyman et al. (1982). The order of preference for independent variables is K_{ow}, S and K_{oc} in descending order.

TOX-SCREEN (USEPA 1984b) a screening-level program for assessing potential fate of chemicals released to the environment, and developed in the Office of Toxic Substances, EPA, uses the regression equation developed by Mackay (1982):

$$BCF = 0.048\, K_{ow} \quad \text{(B-5)}$$

TABLE 30

Recommended Regression Equations for Estimating log BCF, Based on Flow-through Laboratory Studies

Eq. No.	Equation[a]	N[b]	r^2[c]	Chemical Classes Represented	Range of Independent Variable	Species Used
B–13	$\log BCF = 0.76 \log K_{ow} - 0.23$	84	0.823	Wide	7.9 to 8.1×10^6	Fathead minnow Bluegill sunfish Rainbow trout Mosquitofish
B–14	$\log BCF = 2.791 - 0.564 \log S$	36	0.49	Wide	0.001 to 50,000 ppm	Brook trout Rainbow trout Bluegill sunfish Fathead minnow Carp
B–15	$\log BCF = 1.119 \log K_{oc} - 1.579$	13	0.757	Wide	< 1 to 1.2×10^6	Various

a. BCF = bioconcentration factor; K_{ow} = octanol-water partition coefficient; S = water solubility (ppm); K_{oc} = soil (or sediment) adsorption coefficient.
b. N = number of chemicals used to obtain regression equation.
c. r = correlation coefficient for regression equation.
d. In the original equation, the octanol-water partition coefficient was represented by "P" instead of "K_{ow}."
e. The original equation used "WS" (water solubility) instead of "S."

Source: Bysshe (1982)

The estimation methods available are based on regression of data to obtain straight-line correlations. A fair degree of scatter exists in the data. Discrepancies have been found between estimates and laboratory data or field situations. In particular, bioaccumulation of covalently bonded chemicals cannot be predicted by these methods. The estimates provide some means of identifying chemicals which are likely to bioaccumulate in fish and the likely extent of bioconcentration.

The Criteria and Standards Division in the Office of Water Regulations and Standards of the U.S. EPA, in the determination of Ambient Water Quality Criteria, adjusts the equation shown above for lipid soluble compounds. The bioconcentration factor is adjusted for the lipid content of the fish/ shellfish consumed in the diet, as compared to that in the test species, if it was a measured value, or to the species on which estimated values were based. EPA uses a weighted average lipid content of the U.S. fish/shellfish diet of 3% for the protection of human health (USEPA 1980b). For calculating the Final Residue Levels to meet FDA levels, the appropriate lipids value is 100% for fish oil, 11% for freshwater fish and 10% for saltwater species (Stephen et al. 1983). The latter levels are higher because FDA action levels are applied on a species-by-species basis. The highest lipid contents of edible tissue are 11% for freshwater fish (chinook salmon and lake trout) and about 10% for saltwater Atlantic herring.

B.4 PATHWAYS TO CROPS

Very little quantitative guidance (predictive equations and models, etc.) can be provided to assist in assessing the importance of contamination pathways leading to crops. The number of variables is large (crop type, environment, chemical type), and the available data and knowledge are small. In some cases, an order-of-magnitude estimate of the pollutant's concentration in the crop may be made. This may be sufficient for a rough screening of pathways to crops.

Three distinctions are important when assessing pathways to crops:

- Terrestrial vs aquatic environment
- Surface contamination vs uptake
- Organic vs inorganic chemicals

Terrestrial vs Aquatic Environment - Most edible crops are grown in conventional, terrestrial environments (i.e., a field or greenhouse soil plot). These plants "see" two quite different environments: the atmosphere above the soil, and the air/water/nutrient/soil mixture below the soil surface. Uptake of pollutants may differ markedly for these two environments. By contrast, there are plants that grow (or are grown) primarily in an aquatic environment. Examples include algae, seaweed, and some plants grown wholly or partially underwater (e.g., rice).

There is, perhaps, an additional classification for plants grown via hydroponics (i.e., where rooting plants are grown, without soil, in a mineral-rich solution or mist). There should be a special concern for crop contamination in this case for any chemical that is added, or might be added by mistake, to the formulated nutrient solution. In the case of hydroponics and aquatic plants, it may be appropriate to consider the probable (equilibrium) distribution of the pollutant between the aqueous solution (not pure water) and the plant. For neutral organic chemicals it is likely that the plant bioconcentration factor (under these aquatic conditions) will be strongly correlated with the octanol-water partition coefficient and, thus, inversely proportional to water solubility. The correlation equations provided by Baughman and Paris (1981) show this clearly. The lipid content of the plant will clearly have an effect, with higher lipid contents leading to higher bioconcentration factors.

Surface Contamination vs Uptake - A pollutant may easily reach, and adhere to, some surface of a plant (leaf, stem, root), yet not be taken up by the plant. Thus, any crop contamination pathway assessment should clearly distinquish between surface contamination and uptake. The former may be mitigated by subsequent crop washing and processing, the latter might not.

Conventional, terrestrial plants may take up pollutants in three ways: (1) through the stomatal pores of the leaves (foliar uptake); (2) through the stems; and (3) through the roots. For gaseous pollutants released into the air, foliar uptake is likely to be the most important pathway (Vaughan et al. 1981; Guthrie 1980). This may even be the most important pathway for non-volatile pollutants dispersed in the air if the chemical is of moderate to high water solubility and the particles are small enough to penetrate the stomatal pores. In any case, chemicals with high water solubility will be more easily absorbed through the pores into the water-rich plant body.

For pollutants that have become incorporated into the soil, uptake by the roots or tubers may involve more complex processes, especially for ionized species. In this case, especially for inorganic chemicals, there may be relatively little tendency for the plant to accumulate the pollutant to concentrations above that in the surrounding soil. Bioconcentration of neutral organic compounds from soil into plants is still a possibility, but the bioconcentration factors would not be expected to be as large as those found for aquatic biota. This is because soil contains an appreciable amount of organic matter (typically 1-10% by weight in top soils) that will compete as sorption sites for the organic pollutants. In some cases the bioaccumulation factor (concentration in plant/concentration in soil) may be substantially less than 1.0 due to such factors as high soil organic content, high soil adsorption coefficient for the chemical, and the chemical's difficulty in penetrating the root or tuber. For example, a bioaccumulation factor of about 0.001 was found for corn (*Zea mays*) grown in soil contaminated with up to 20,000 mg/kg di-n-butyl phthalate (Shea et al. 1982).

Organic vs Inorganic Chemicals - A number of distinctions have already been made with regard to organic vs inorganic chemicals and the associated difference in plant uptake. It is worth repeating here, however, the general admonition to consider the chemical nature of the pollutant in assessing the potential uptake by crops. The specific considerations should include, for example:

- water solubility
- dissociation in water (speciation)
- octanol-water partition coefficient
- soil adsorption coefficient
- reactivity in solution (e.g., oxidation, reduction, complexation, and precipitation of metals; hydrolysis, oxidation, biodegradation of organics)
- volatility (including Henry's law constant)

The pathways to crops are assessed by two separate routes: uptake from air and uptake from roots. Depending on the properties of the chemical and the nature of release of the chemical, one or both of these routes may be important.

B.4.1 Foliar Uptake from Air

As a very crude theoretical estimate, plant tissue may be considered to be a reservoir of water contained by a sheath that is permeable to the chemical. The uptake from air may be approximated by the use of the chemical's Henry's law constant (H).

$$C_p = \frac{C_a RT}{H} \qquad \text{(B-6)}$$

Where:

C_p = concentration of pollutant in plant (ug/ml)

C_a = concentration of pollutant in air (ug/ml)

H = Henry's Law Constant (m^3 atm/mol)

R = gas constant (8.2×10^{-5} m^3 atm/mol °K)

T = temperature (°K)

This method could overestimate the absorption of a chemical into foliar solution because the latter is not pure water and the solubility of the chemical in it could be lower than in pure water. In addition, the action of the cuticle as a barrier is ignored. On the other hand, there may be a favorable partition of a chemical into plant solution if the chemical is more soluble in the plant solution than in water.

As an example, assume a plant is exposed to contaminated air containing 0.001 ug/ml methylene chloride. Since H for methylene chloride (@ 25°C) is about 3×10^{-3} atm m^3/mol, the equilibrium concentration in pure water is about 0.01 ug/mL.

The model used by TOX-SCREEN (USEPA 1984b) is an interception model developed by Chamberlain (1970). This model and suggested parameters are shown in Table 31. A factor, T_v, has also been included in some models (USEPA 1984c) to relate radionuclide concentration in the edible portion of a crop to that calculated in the equation shown in Table 27. Baker et al. (1976) suggested a value of 1.0 for leafy vegetables and fresh forage, and 0.1 for all other produce. A factor of 1.0 should probably be used for a conservative approach.

TABLE 31

CONCENTRATION OF COMPOUND IN PLANTS AS A RESULT OF INTERCEPTION

$$C_p = \frac{r}{Y_v \quad \lambda_{ei}} \left[1 - \frac{1 - e^{-\lambda_{ei} t_e}}{\lambda_{ei} t_e} \right] \text{x [deposition rate]}$$

where

C_p = concentration of pollutant in plant (ug/g)

r = empirically determined initial interception fraction

Y_v = vegetative productivity (g/m^2)

λ_{ei}= empirical weathering constant (day^{-1})

t_e = crop growth period before harvest or grazing (days) deposition rate in g/m^2-day.

Values

r/Y_v = average of 2.0 m /kg for grasses based on a dry-weight value of Y_v of about 0.1 kg/m^2 (Chamberlain, 1970)

r = 0.25 for deposition of radionuclides on pasture (USNRC 1977)

= 0.4 may be more appropriate for organics than values above (Morton et al. 1967)

Y_v = 0.7 kg/m^2 fresh weight for radionuclides on pasture (USNRC, 1977)

= 0.15 kg/m^2 default value

λ_{ei} = 0.05 day^{-1}(Chamberlain 1970; USNRC 1977), value probably smaller for organics

t_e = 30 days for grasses (USNRC 1977)

Source: USEPA (1984b,c)

B.4.2 Root Uptake

Briggs et al. (1982) used a Root Concentration Factor (RCF) and a Transpiration Stream Concentration Factor (TSCF) to describe uptake into roots and subsequently into shoots.

RCF = (concentration in roots)/(concentration in external solution) (B-7)

TSCF = (concentration in transpiration stream)/(concentration in external solution) (B-8)

The RCF is generally independent of concentration for dilute solutions and the TSCF has a maximum value of 1.0 for passive uptake. The regression equations obtained for 18 compounds (non-ionic o-methylcarbamoyloximes and substituted phenylureas) in barley shoots are as follows:

$$\log (\mathrm{RCF} - 0.82) = 0.77 \log K_{ow} - 1.52 \quad \text{(B-9)}$$

$$\mathrm{TSCF} = 0.784 \exp - [(\log K_{ow} - 1.78)^2/2.44] \quad \text{(B-10)}$$

$$\mathrm{RCF} = 0.82 \text{ (for polar species)} \quad \text{(B-11)}$$

The measured value of the TSCF for 3-(methylthio)phenylurea was much less than its predicted value. The regression equations above will not provide accurate values, but appear to apply reasonably well to some crop species including rice, lettuce, turnip, and wheat. Root physiology or rapid metabolism in roots, e.g., in carrots or parsnips, may reduce translocation, leading to higher predicted TSCF values than would be measured.

The regression equations by Briggs et al. (1982) were obtained from experiments with barley shoots in nutrient solutions. For plants in soil, the concentration of a chemical in the soil solution may be estimated by:

$$C_s = \frac{C_o}{K_d} \quad \text{(B-12)}$$

where:

C_s = concentration in soil solution (g/ml)

C_o = total concentration in soil (g/g)

K_d = bulk soil partition coefficient

For compounds whose partitioning is governed largely by organic matter, the soil solution concentration can be estimated as follows.

$$C_s = \frac{C_o}{K_{oc}\,(\mathrm{OC})} \quad \text{(B-13)}$$

where:

OC = the fractional organic carbon content (g/g)
K_{oc} = Organic carbon adsorption coefficient (ug/g / ug/ml)

Redefining, RCF_s = (concentration in roots)/(total concentration in soil)
$TSCF_s$ = (concentration in transpiration stream)/(total concentration in soil)

we obtain:

$$\log [RCF_s K_{oc} (OC) - 0.82] = 0.77 \log K_{ow} - 1.52 \qquad (B\text{-}14)$$

$$TSCF_s K_{oc} (OC) = 0.784 \exp - [(\log K_{ow}-1.78)^2/2.44] \qquad (B\text{-}15)$$

$$RCF_s \ K_{oc} (OC) = 0.82 \text{ (for polar species)} \qquad (B\text{-}16)$$

The work of Briggs et al. (1982) is incorporated into the Pesticide Root Zone Model (PRZM). This model simulates the vertical movement of pesticides in the unsaturated zone. Various processes are incorporated into the model, including plant uptake. The model uses an uptake efficiency factor calculated using Equation B-10 (Carsel et al. 1984). However the use of these equations for compounds and concentrations outside the range tested by Briggs et al. (1982) may produce questionable estimates. Experimental data for DDT from Nash et al. (1970) and Onsager et al. (1970) were substantially lower than levels predicted using Equation B-14.

In TOX-SCREEN (USEPA 1984b) the relationship used was between K_d (soil-water partition coefficient) and a bioconcentration factor, BC_{pl}, defined as the ratio of the mature plant parts concentration of a chemical (ug/g dry weight) to the soil concentration (ug/g dry weight).

$$C_{pl} = BC_{pl} \times C_o \qquad (B\text{-}17)$$

K_d is related to K_{oc} approximately by:

$$K_d = K_{oc} \times (OC) \qquad (B\text{-}18)$$

The regression equation used in TOX-SCREEN for radionuclides was developed by Baes (in press) and is as follows:

$$\ln K_d = A+B \ln (BC_{pl}) \qquad (B\text{-}19)$$

or $$\ln [K_{oc} \times OC] = A+B \ln (BC_{pl}) \qquad (B\text{-}20)$$

The values used for A and B in TOX-SCREEN are 3.02 and -0.85, respectively, derived from a literature review of 21 elements.

B.5 PATHWAYS TO FOOD--POST-HARVEST STAGES

There are four major pollutant food chain "access points" in the post-harvest stages: (1) Food in contact with air (2) Food in contact with water or another liquid, (3) Food to which something is added and, (4) Food in contact with a surface. Relevant or significant pollutant pathways in the environment have been identified and discussed in

Sections A-3 and A-4. These pathways eventually involve contact of the food or feed with one or more of the above media.

For all of these pathways, food contamination can occur via a number of pollutant pathways in the food matrix. A food matrix will consist, in general, of one or more homogeneous phases. The phases are food-air, food-water, and food-solids, as shown in Figure 8. This figure shows that a substance can diffuse from external air to food air (Pathway 1), or from external liquid to food liquid (Pathway 2). Once in the food, the pollutant can be partitioned between the phases within the food matrix. The following sections consider contamination via the four access points, considering the different pathways in the food matrix as appropriate.

B.5.1 Food in Contact with Air, Water or Liquid

It is documented that pollutants can migrate from air, water, or other liquid designated as "external" media -- into food in a variety of situations (see Table 15) and in a number of post-harvest stages. The situations of contact are numerous, but the mechanisms -- and governing algorithms -- of pollutant migration are similar in many cases. The rate and extent of migration are dependent on a multiplicity of factors, including pollutant concentrations in the external media, pollutant characteristics, time of food exposure, food characteristics, and temperature.

In the following analysis, it is assumed that a pollutant is uniformly present in the external media of the food, and that the food is impacted by a constant concentration unless stated otherwise. In that respect, contamination of the food may take place (Morrill et al. 1982) as a result of two sequential major processes:

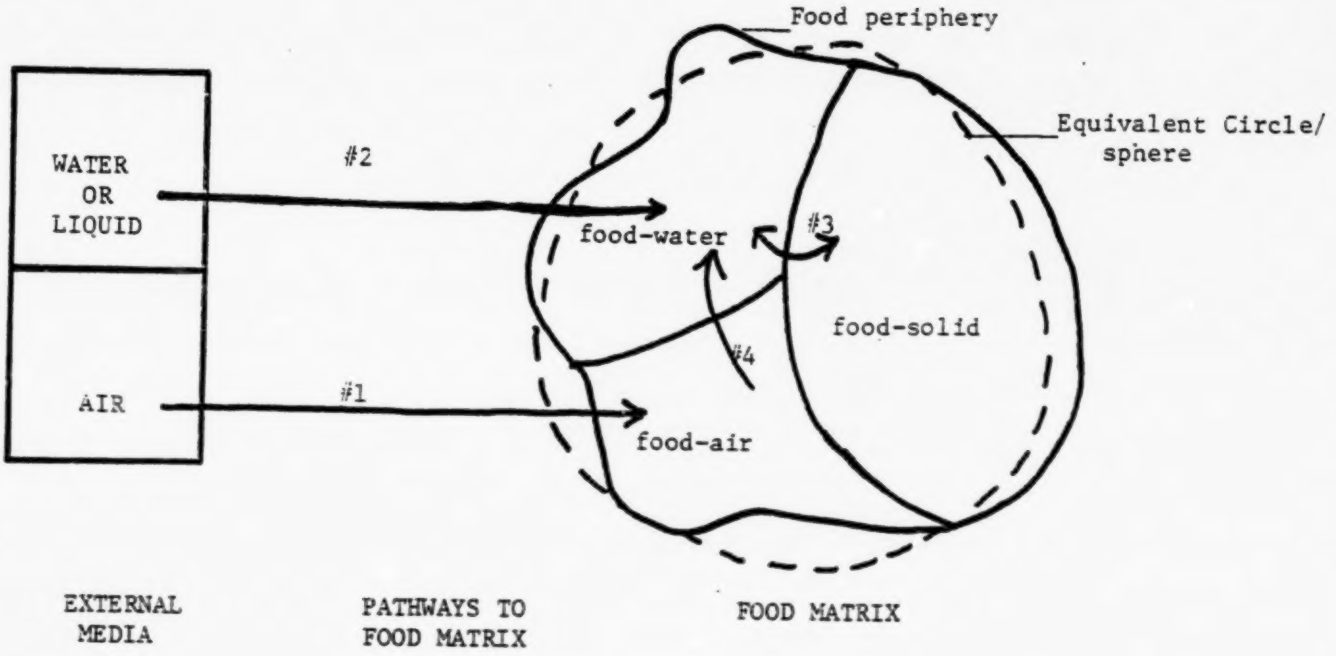
(1) Diffusion of the pollutant (from the air or water) through the surface of the food into the food moisture (water), the food-air, or the food-solid as a result of a concentration gradient between the external media and the food,

(2) Partitioning of the pollutant molecules into the various phases of food, either by adsorption or dissolution in the organic fraction of the food.

The above processes are time and temperature dependent, but in the following section, only steady-state and temperature independent conditions are described. When necessary, however, a separate discussion on the effects of these parameters is given.

B.5.1.1 Diffusion

For non-homogeneous foods, like an apple or a piece of meat, diffusion of the pollutant may have to take place through more than one layer, for example through both the apple peel and the apple body. In addition, diffusion can take place across any section of different media, for example, from the air of an external medium to the air of the food pores, or from the air of an external medium to the moisture of the food.


Food periphery
Equivalent Circle/ sphere
WATER OR LIQUID
AIR
#2
#1
food-water
#3
#4
food-solid
food-air
EXTERNAL MEDIA
PATHWAYS TO FOOD MATRIX
FOOD MATRIX

# 1 External air to food air
# 2 External water or liquid to food moisture
# 3 Food water to food solid
# 4 Food air to food water

FIGURE 8 SCENARIOS OF FOOD CONTAMINATION

The mass of a diffusing pollutant along a direction (x) and passing through a given cross section per unit time is described by Fick's first law, which says that the pollutant flux is directly proportional to the concentration gradient:

$$F = - D\ (dc/dx) \qquad \text{(B-21)}$$

where:

F = pollutant mass flux along a direction x (ug/cm^{2}s)
D = diffusion coefficient of pollutant in the food phase (cm^2/s)
c = concentration of pollutant in a medium (ug/ml)
dc/dx = concentration gradient in direction x

Equation B-21 applies to all media and any type of diffusion process (e.g., air-to-air, air-to-moisture) and represents the basic equation for estimating pollutant migration into food from air, water or liquid (external media). Although diffusion can occur in all three phases (air, moisture, solids) of a food piece; it takes place most rapidly in the food-air, and least rapidly in the food-solids. In general, diffusion of contaminants in the vapor phase (air) occurs 10^4 times faster than in water. Diffusion in the solid phase may be very slow compared to other pollutant transport processes. The same principle can be assumed to apply in food, therefore, diffusion in solids is neglected in the sections to follow.

B.5.1.1.1 Diffusion from Air to Food Air

The Farmer formula for estimating pollutant flux from soil-air to the air is adapted for spherical (or circular) food pieces:

$$F_1 = D_{fa}^{*}\ (C_a - C_{fa})/r \qquad \text{(B-22)}$$

where:

F_1 - pollutant mass flux across food surface in pathway #1 in Figure B-1 (ug/cm^{2}s);

D_{fa}^{*} - apparent diffusion coefficient of pollutant in food air (cm^2/s);

C_a - concentration of the pollutant in the air (external medium) of the food (ug/cm^3)
C_{fa} - concentration of the pollutant in the food air (ug/cm^3)

r - approximate radius of the food piece as shown in Figure B-1 (cm).

For a particular pollutant, the apparent diffusion coefficients may be required for food-air (D_{fa}^{*}) and food-moisture (D_{fm}^{*}). An apparent diffusion coefficient accounts for the reduction in the rate of diffusion due to the particles of the food substance. The estimation of both apparent diffusion coefficients is discussed in Bonazountas and Wagner (1981). A brief discussion is included here. Apparent diffusion coefficients can be estimated from food porosity via the relationship Millington and Quirk (1961) developed for porous media, principally soils:

$$D_{fa}^{*} = D_a (n_{air}^{10/3}/n_f^2) \qquad \text{(B-23)}$$

where:

D_{fa}^{*} = apparent diffusion coefficient of compound in food-air (cm^2/s);
D_a = diffusion coefficient of compound in vapor (air) (cm^2/s);
n_{air} = food-air-filled porosity (ml/ml);
n_f = food (total) porosity (ml/ml)

The food-air-filled porosity (n_{air}) in equation (B-23) can be estimated from the (total) food porosity (n_f) and the food water content m (ml/ml):

$$n_{air} = n_f - m \qquad \text{(B-24)}$$

Food porosity is not a commonly reported parameter, however, it may sometimes be found in the literature. For example, Roman et al. (1979) reported a porosity of 0.225 for apples. The diffusion coefficient for the pollutant in air (D_a) must also be obtained in order to use equation B-27. It is not expected that these would generally be available. Such coefficients can, however, be estimated using the methods described in Tucker and Nelken (1982). The duration of time that a food particle is exposed to contaminated air is dependent on the processing of the food. For example, air is blown onto fruits to separate them after harvesting. Each fruit may only be exposed to the air for a brief period of less than an hour. On the other hand, storage of the fruit in a warehouse which has been sprayed with a pesticide will expose the fruit for a longer period of time. The mass and surface area of the food piece exposed depends on the type of food, the processing method, and the processing stage.

Additional relationships between diffusion coefficients and temperature or pressure have been developed for soils by Farmer et al. (1980) and Hamaker (1972) and could probably be employed in this type of analysis if desired. In general, however, equations B-22 and B-23 should be used with caution, since their validity for food is uncertain.

The flux (F_1) is a function of the concentration in the food air, C_{fa}, and of time. In order to present this variable rate for a non-contaminated food piece, an average flux rate $\overline{F}_1$ is used.

$$\overline{F}_1 = F_1/2 \text{ for } C_{fa} = 0 \text{ at } t=0 \qquad \text{(B-25)}$$

While an exponential function could be used to estimate a flux F_1, the rate constant is unknown, and it would be necessary to calculate it iteratively over time. As a simplication, it was assumed that the use of an average flux would provide an adequate representation of the system.

Once $\bar{F}_1$ has been estimated, the pollutant concentration in the food can be estimated from:

$$C_t = C_i + (\bar{F}_1 A t)/M \tag{B-26}$$

where

C_t = concentration of the pollutant in the food after time t (ug/kg)
C_i = initial pollutant concentration in food (ug/kg)
F_1 = average pollutant mass flux across food surface (ug/cm^2 s)
t = time (s)
M = mass of food piece (kg)
A = surface area of the food piece (cm^2)

This method estimates an average concentration in the food. The concentration at various points in the food piece will vary, however, depending on the time exposed. In addition, for the irregularly-shaped food piece, a radius can be calculated assuming a spherical piece of equal volume.

This model does not consider the deposition of particulates, which would largely depend upon particle size. Once deposited on the food, the chemical may be absorbed. This could occur through solubilization or volatilization and diffusion into the food item. For methods of estimating uptake from particulate deposition, see Section B.4.1.

In addition, this model considers diffusion through air spaces in the food to be the only mechanism for absorption from air. It is unknown how accurately this may represent the actual case. It is presented here as a first attempt at representing the diffusion of vapors in food pieces.

B.5.1.1.2 Diffusion from External Liquid to Food Liquid

Equations similar to the equations above may be used for liquid-to-liquid diffusion:

$$F_2 = D_{fm}^{*} (C_{el} - C_{fm})/r \tag{B-27}$$

where:

F_2 = pollutant mass flux across food surface in Pathway 2 (ug/cm^2 s);
D_{fm}^{*} = apparent diffusion coefficient in food moisture (cm^2/s);
C_{el} = concentration of the pollutant in the external liquid medium (ug/ml);
C_{fm} = concentration of the pollutant in the food moisture (ug/ml)
r = approximate radius of food particle (cm)

Equations to estimate apparent diffusion coefficients, average flux, and concentration in food after time t, are similar to those above for air-to-air diffusion.

B.5.1.2 Partitioning

A food matrix may consist of three phases: Food-air, food-moisture, or water, and food-solids. A pollutant impacting a food matrix can be "partitioned" and the pollutant can be present in all three phases: mixed in food-air, dissolved in food-moisture, or sorbed on food particles. The equilibrium concentration of the pollutant in each phase can be related to the equilibrium concentration of the same pollutant in the other phases via partition coefficients. As a result, partition coefficients may be derived for pollutants in the various phases (e.g., in the air as the external medium and the food-air, the food-air and the food-moisture, the food-moisture and the food-solids).

Partition coefficients are derived from laboratory experiments conducted under constant temperature and primarily for pollutants partitioning between liquid (moisture) and solid phases in a porous medium (i.e., adsorption experiments). The experimental results lead to formulation of partitioning, isotherm, or adsorption equations.

B.5.1.2.1 Moisture-Solid Partitioning

The moisture - solid partitioning coefficient often used is the Freundlich isotherm expressed by:

$$s = x/M = KC_{el}^{1/n} \qquad \text{(B-28)}$$

where:

s = adsorbed concentration of contaminant on food particles; (ug/g food)
x = adsorbed pollutant mass on/in food; (ug)
M = mass of food; (g)
K = adsorption (partitioning) coefficient; (ug/g)/(ug/ml)
C_{el} = dissolved concentration of pollutant in external liquid; (ug/ml)
n = Freundlich isotherm parameter.

Equation (B-28) can also be used for internal partitioning between any two phases (e.g., pathway #3, Figure 8).

B.5.1.2.2 Moisture-Air Partitioning

The moisture-air partitioning coefficient used is the Henry's law Constant, expressed by:

$$C_{fa} = C_{fm} \, H/RT \qquad \text{(B-29)}$$

where:

C_{fa} = concentration in food-air (ug/ml);

C_{fm} = concentration in food-moisture (ug/ml);

H = Henry's law constant (m^3 atm/mol);

R = gas constant (8.2×10^{-5} m^3 atm/mol. °K)

T = temperature (°K).

B.5.1.2.3 Partitioning Coefficient, K

The value of the partitioning (adsorption) coefficient K of equation (B-28) can be measured in laboratory experiments. Food/water partition values, however, are not commonly reported in the literature. Of the more common solvents, n-octanol is believed to best imitate the lipid content in plants (Kenaga and Goring 1980). Therefore, partitioning may be estimated from an octanol/water partitioning coefficient (K_{ow}) and the relationship:

$$K = K_{ow} \text{ (\% lipid)}/100 \qquad \text{(B-30)}$$

The above equation has been adapted from a similar equation derived for organic soils, which may have an organic content of 0.2-6%. In comparison, Table 32 summarizes the components of various food items. Note that the organic content of foods spans a much wider range than does the organic content of soil.

The above equation assumes equilibrium conditions, and that the surface area of the food is equivalent to that of soil particles for which the K_{ow} is measured. This may be a reasonable assumption for small food particles, but may have to be corrected for larger chunks of food with a low surface/volume ratio.

B.5.1.3 Application of Methods

The above sections have presented a variety of equations that purport to represent pollutant migration. It is assumed that they apply to food, since they have been shown to apply to other porous substances. However, the validity of these models is unknown for the situations described above.

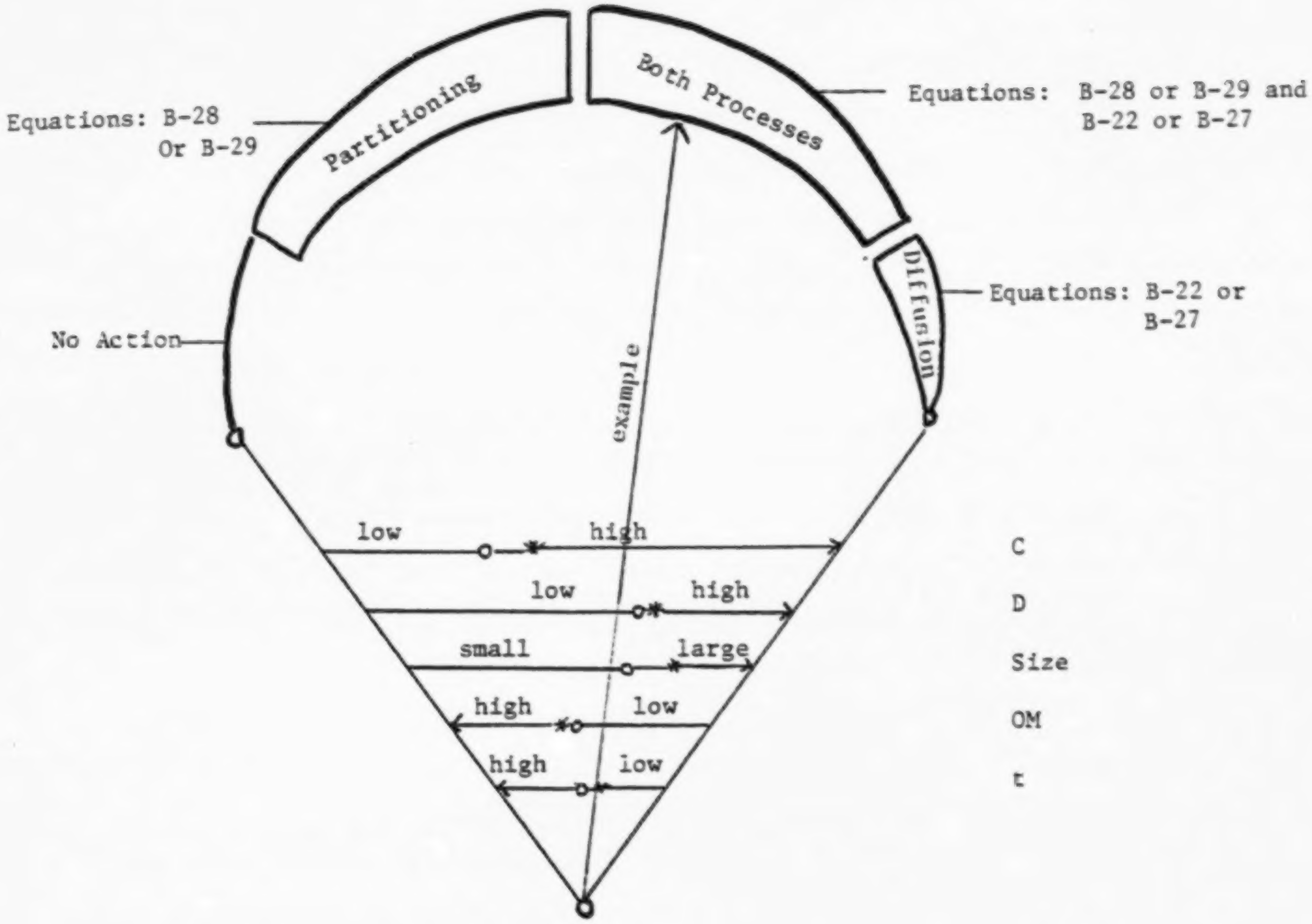
Independent equations for diffusion and partitioning have been described, when, in fact, they are interrelated. Figure 9 shows how to apply the various equations described above. These terms are all relative, and will take some practice to determine the best methods to use. This diagram is intended to indicate that if the size of the food piece is small, and the time is large, partitioning assumptions can be used. If the time of contact is short and the food piece is large, diffusion considerations are more appropriate. The concentration of the pollutant in the external medium, the apparent diffusion coefficient in the food, and the organic content of the food must also be considered in choosing the most appropriate method.

TABLE 32

WATER, PROTEIN, FAT, AND CARBOHYDRATE DISTRIBUTION OF FRESH UNCOOKED FOODS

	Approximate Range of Composition (%)			
Food Group	Water	Protein	Fat	Carbohydrate
Grain and legume seeds	11-12.6	7.5-23.8	1-1.8	59.4-78.8
Fatty nuts	2.6-5.3	3.4-26.9	34.5-73.0	11-23.6
Vegetable--green foliage, stems, roots	74-94	0.1-7.5	0.2-1.4	2.9-31.2
"Juicy" fruit (pome, citrus, berries, etc.)	74-94	0.3-1.4	0.1-1.4	4.0-14.9
Fatty, juicy fruits (coconut and avocado)	45-67	1.7-3.4	26.4-34.7	5.1-14.0
Meat (beef,pork)	33-71	9-21	6-66	0
Poultry	66-77	16-30	2-18	0
Fish	72-81	17-30	0.1-8	0
Seafood	78-85	9-18	0.2-2	0.5-3

Source: Kenaga (1975, adapted from Spector 1956) and USDA (1975)


Equations: B-28
Or B-29
Partitioning
Both Processes
Equations: B-28 or B-29 and
B-22 or B-27
Diffusion
Equations: B-22 or
B-27
No Action
example
low
high
C
low
high
D
small
large
Size
high
low
OM
high
low
t

Given

C: External medium concentration = high-to-low
D: Apparent diffusion coefficient (compound/food piece) = high-to-low
Size: Size of food piece = small to large
OM: Organic matter content of food = high-to-low
t: Time of food exposure to C = low-to-high

Example (indicated by *)

FIGURE 9 EVALUATION OF NUMERICAL ESTIMATION PROCEDURES FOR FOOD POST-HARVEST (DIFFUSION VS. PARTITIONING)

B.5.2 Food in Contact with Surfaces

Food may contact various surfaces, including harvesting equipment, preparation or storage surfaces, and packaging. The potential for contamination occurring via these pathways depends upon the likelihood of the chemical migrating out of the material contacting the food, and the propensity of the food for taking it up. These issues are described in detail in a methodology for estimating migration rates of additives and impurities from porous materials (Schwope et al. 1984). This methodology was specifically designed for the migration of pollutants from polymeric materials. These substances would commonly contact food, but the methodology may apply to other porous materials as well.

The maximum amount of chemical (g/cm^2) that could migrate out of a porous surface at any time, t, is given by:

$$M_t = 2\, C_{op}\, (D_p t/\pi)^{1/2} \qquad \text{(B-31)}$$

where:

M_t = amount migrated at time t (g/cm^2)
C_{op} = initial chemical concentration in surface (g/cm^3)
D_p = effective diffusion coefficient through surface (cm^2/sec)
t_p = time of contact of food with surface (sec)

The effective diffusion coefficent, D_p, may be calculated using equation B-23 in Section B.5.1.1.1. Assuming that all the migrated chemical enters the food particle, the average concentration in the food is given by:

$$C_f = 2C_{op}\, (D_p t/\pi)^{1/2}\, A_f/V_f \qquad \text{(B-32)}$$

where:

C_f = average concentration of chemical in food (g/cm^3)
A_f = surface area of food in contact in the surface (cm^2)
V_f = volume of food (cm^3)

The concentration of chemical in the food is limited by the equilibrium partitioning between the food and the surface, which may be estimated by equation B-28 in Section B.5.1.2.3.

B.5.3 Additives

The addition of pollutants to food may occur directly, for example, as a food additive. In addition, water or air containing the pollutant may be added to the food. In either case, the resultant concentration in the food is easily calculated if the concentration of the pollutant in the substance being added (C_a) and the mass of the substance being added (M_a) are known. The calculation is as follows:

$$C_f = C_i + \frac{C_a M_a}{M_f + M_a} \qquad \text{(B-33)}$$

where:

C_f - the final concentration of the pollutant in the food (ug/kg);
C_i - the initial concentration of the pollutant in the food (ug/kg);
C_a - the concentration of the pollutant in the substance being added to the food (ug/kg);
M_a - the mass of the substance being added (kg);
M_f - the mass of the food to which the substance is added (kg).

B.6 CHEMICAL LOSSES

B.6.1 Potential Pathways of Pollutant Loss

Previous sections of the report have concentrated on the identification of pathways of food contamination and the presentation of quantitative methods for assessing these pathways. The intent was to provide methods for determining a chemical's potential for food contamination. The implicit assumption has been that if a food item is contaminated at one stage, that pollutant persists at the same concentration and in the same form until it is consumed. Obviously this is not a realistic assumption, although it provides a simple means of estimating exposure. Pollutants can be lost or degraded in food during the same stage in which they are contacted, or in subsequent stages. In fact, these losses can be quite substantial. Ferreira and Seiber (1981) reported about 36% loss by root exudation, and 6% by volatilization from rice plants that had been systemically treated with carbofuran. Table 33 shows losses of some pesticides from spinach in washing and blanching. These results suggest that losses can be great. However, these situations represent a foliar application of a pesticide, and probably largely surface contamination. Similarly, peeling has been shown to decrease pesticide residues up to 90% (Geisman 1975). However, if the pollutant is taken up through the roots, surface treatments (i.e., washing and peeling) are not likely to have a significant effect on residues.

Chemical losses from food have been considered to a large extent in the context of vitamin loss or the reduction of pesticide residues (Geisman 1975; Lund 1975; Krochta and Feinberg 1975). While this work provides insight into the possible pathways of pollutant loss, the sources of contamination and the chemical properties may be different for many other compounds. Table 34 shows the potential pathways for pollutant losses from food. The relative importance of these pathways depends upon the type of food, the conditions, and the physical and chemical properties of the chemical.

B.6.2 Methods for Assessing Chemical Losses From Food

Most of the methods discussed in Section B-5 describing migration of contaminants into food can be utilized to assess losses. In the case of diffusion, the concentration gradient would force movement of the pollutant from the food. Where partitioning or equilibrium conditions are utilized, movement in both directions is assumed. The pathways of loss for which no methods are available are those involving chemical degradation. Thermal degradation appears to be an important loss

TABLE 33 REMOVAL OF PESTICIDE RESIDUES FROM SPINACH BY BLANCHING AND WASHING PLUS BLANCHING

Compound	Removal (%) by	
	Blanching	Washing and Blanching
DDT	48	60
Carbaryl	84	97
Parathion	61	71

Source: Farrow et al. 1969

TABLE 34 PATHWAYS OF POLLUTANT LOSS FROM FOOD

Stage	Loss Pathway
Food Generation Stages	
Plants	Guttation and volatilization
	Root exudation
	Photolysis
	Metabolism
Animals	Metabolism
Post Harvest Stages	
Plants	Volatilization
	Thermal degradation
	Leaching (diffusion)
	Physical - peeling, trimming
Animals	Volatilization
	Thermal degradation
	Leaching (diffusion)

mechanism for some chemicals (Geisman 1975). Empirical models have been developed to predict loss of some chemicals in food. For example, Williams and Nelson (1974) presented rate constants for the thermal degradation of methylmethionine sulfonium ions (precursor of dimethyl sulfide) in sweet corn and tomatoes, and Wanninger (1972) predicted the stability of ascorbic acid in food products. However, these models have empirically-derived rate constants and are not generalizable for other chemicals.

APPENDIX C
EXAMPLE OF PATHWAYS APPROACH AND QUANTITATIVE METHODS

C.1 INTRODUCTION

This appendix describes the application of the pathways identification methodology and quantitative methods from Appendices A and B, respectively, to benzanthrone. The other parts of the overall methodology to assess dietary intake are described in Section 4.0. The application of the pathways identification methodology (Step 3 of the overall methodology) will be described first. The relevant quantitative methods (Step 4 in the overall methodology) are then applied to the significant pathways from the pathways methodology.

C.2 PATHWAYS IDENTIFICATION METHODOLOGY

Chemical - Benzanthrone

Production - Benzanthrone is produced by up to 6 companies in eight locations. The current production volume is unknown, but was 376 kkg in 1974.

Uses - The primary use of benzanthrone is as an intermediate in the production of dyes. It is also used to manufacture 3-methoxybenzanthrone, which is used as a luminophore.

Important Properties

Water solubility	1.5×10^{-5} moles/L
Vapor Pressure	6.9×10^{-10} mm Hg @ 25° C
Physical State at Room Temperature .	Solid
Log K_{ow}	3.88
Henry's Law Constant	6.0×10^{-11} atm m^3/mol
Soil Adsorption Coefficient (K_{oc})	3700
Bioconcentration factor (fish)	523

C.2.1 Identify Situations of Release

Since the chemical is used only as an intermediate, releases would be largely from production facilities, the locations of which are known. Locations where it may be used in the production of dyes are unknown. For the purposes of an example it was assumed that the chemical is released to surface waters in the vicinity of production facilities, resulting in a concentration of about 10 ug/L in surface water. No other situations of release are expected for this chemical. The low vapor pressure of benzanthrone suggests that releases to air would not be significant. In addition, the extremely low Henry's Law constant suggests that volatilization from water would be unimportant.

C.2.2 Identify Situations of Direct Contact or Addition

No situations of direct contact are anticipated for this chemical since it is not used as a food additive in any of the food chain access stages.

C.2.3 Identify Pathways for Indirect Contamination Routes

An examination of Table 17 shows the various pathways of food contamination which can result upon release to ambient waters. While the locations of the production facilities are known, the identification of uses of receiving waters for fishing, irrigation or as a drinking water supply for livestock and poultry is not easily accomplished. Therefore, since the pathways were limited by the types of release, it was thought useful to include as relevant all pathways originating from contaminated surface waters. The relevant contamination pathways are shown in Table 35.

C.2.4 Identify Most Significant Pathways

A prioritization scheme for relevant pathways is found in Table 23. Since an estimate of the concentration of benzanthrone in ambient water is available, this scheme can be started at (4) Mobility from compartment to food. Table 36 shows the scorings for the relevant pathways. While this table is done on a very subjective basis, it does provide a framework for prioritization. The ingestion of drinking water by poultry and livestock is shown as a more significant pathway than the others, as the octanol-water partition coefficient is greater than 3.5, suggesting that the substance may bioaccumulate in animals (Garten and Trabalka 1983). The bioconcentration factor in fish is not particularly high, thus the score of 2 for mobility. Uptake from irrigation water was thought to be limited, due to the low solubility and the high adsorption coefficient. Adsorption to soils may, however, be important. Food in the post-harvest stages was scored as a 3 because in some cases the water may be a component of the food item. All pathways received a score of 2 for the number of steps because the compound was directly released to water which contacted food in some form.

The amount of food contaminated cannot be evaluated at this point in the analysis as described above in C.2.3. Thus, the most significant pathways appear to be ingestion of drinking water by livestock and poultry, the contamination of food in the post-harvest stages by processing water which may contact or be incorporated into the food item, and absorption from ambient water by fish.

C.3 QUANTITATIVE METHODS

Estimation methods may be applied to each of the significant pathways identified above.

C.3.1 Ingestion of Drinking Water By Livestock and Poultry

The screening value discussed in Appendix A of $K_{ow} = 3.5$ suggests that this pathway can justifiably be identified as significant. The equation for estimating pollutant concentration in edible tissue is:

$$C_T = BF_f \, (F) \, C_D$$

Using the method of Kenaga (1980) and a log K_{ow} of 3.88,

TABLE 35 RELEVANT CONTAMINATION PATHWAYS FOR BENZANTHRONE

Source of Human Exposure	Pathway of Contamination
Meat - beef dairy cows hogs and pigs sheep and lamb poultry	ingestion of drinking water dermal absorption from water
Fish	absorption from water
Plant - field crops vegetables berries orchard fruits	uptake from irrigation water
Food Post Harvest	absorption/addition of water used in processing

TABLE 36 SCORING OF RELEVANT CONTAMINATION PATHWAYS FOR BENZANTHRONE

Source of Human Exposure	Pathways	Score		
		Mobility to Food	Number of Steps	Total
Beef	Ingestion of drinking water	3	2	5
Dairy	"	3	2	5
Hogs and Pigs	"	3	2	5
Sheep and Lamb	"	3	2	5
Poultry	"	3	2	5
Fish	Absorption from water	2	2	4
Field crops	Uptake from irrigation water	1	2	3
Vegetables	"	1	2	3
Berries	"	1	2	3
Orchard Fruit	"	1	2	3
Food Post Harvest	absorption/addition of water used in processing	3	2	5

$$\log BF_f = -3.457 + 0.500 \log K_{ow} = -1.5$$
$$BF_f = 0.03$$

Assuming a fat content in beef of 15%

$$C_T = 0.03\ (0.15)\ (10)$$
$$= 0.045\ \text{ug/kg in beef.}$$

The screening level of Garten and Trabalka (1983) is log $K_{ow} < 3.5$ for no appreciable bioaccumulation. The value calculated above shows very little bioaccumulation in beef, which is consistent with this screening level.

Such an estimation involves numerous assumptions. The first assumption is that the animal consistently receives drinking water containing 10 ug/L. In addition, the use of Kenaga's method has limitations, as discussed in Appendix B. It is not recommended, but is included here only as an example of the method. It is rarely likely that BCF_f values for livestock and poultry will be available, and concentrations resulting in these organisms cannot generally be estimated. These BCF_f values are well correlated with those in rodents, so that such values obtained in the laboratory may be used when available.

C.3.2 Food -- Post-Harvest

The manufacture of beverages probably represents the largest source of direct addition of water in food processing operations. In addition, Table 23 suggests that bottling operations are prevalent in the U.S. Since soft drinks, coffee and tea are 90-100% water, concentrations close to 10 ug/L would remain in these beverages, assuming no losses. Other items such as bread, rice, etc. incorporate water, but concentrations would not generally be as high.

The use of process water containing benzanthrone could also result in food contamination. Since no information was available on the types of food potentially contaminated, apples soaking in water were chosen as an example.

Apples contact water frequently during processing and transport in the plant as described in Perwak et al. (1981a) and in Tables 15 and 16. It is assumed here that an apple is totally immersed in water for 1 hour. Section B.5.1.1.2 describes the estimation methods available for such a situation. Figure 9 displays the various processes which may be assessed. An hour seems a short time and the food piece is relatively large, thus diffusion would seem the more appropriate process to model. However, for the purposes of example, partitioning will be considered as well. Consider the flux from the liquid into the food as follows:

$$F_2 = D_{fm}^{*}\ (C_{el} - C_{fm})/r$$
$$= D_{fm}^{*}\ (0.01)/5$$
$$= D_{fm}^{*}\ 0.002\ \text{ug/cm}^2\ \text{sec}$$

where $C_{fm} = 0$ and $r = 5$ cm.

The apparent diffusion coefficient in food moisture D_{fm}^* is related to the diffusion coefficient in water (D_w). This equation is used for calculating D_{fm}^*, although its applicability is unknown.

$$D_{fm}^* = D_w \,(n_{wat}^{10/3}/n_f^{\,2}) \quad cm^2/s$$

The total porosity (n_f) of an apple is estimated to be 0.3. (Roman et al. 1979) The water-filled porosity n_{wat} is expected to be close to that and assumed tc be 0.25. In addition, Schwope et al. (1984) showed that D_w is related to a compound's molecular weight. D_w for benzanthrone (mol. wt. 230) can be estimated by:

$$D_w = 2.5 \times 10^{-5}/\,MW^{1/6} \quad cm^2/sec$$
$$= 1 \times 10^{-5} \quad cm^2/sec$$

The effective diffusivity is estimated by:

$$D_{fm}^* = 1 \times 10^{-5}\,((0.25)^{10/3}/\,(0.3)^2) \qquad cm^2/sec$$
$$= (9.8 \text{x} 10^{-3}/0.09) \times 10^{-5} \quad cm^2/sec$$
$$= 1 \times 10^{-6} \; cm^2/sec$$

Therefore, $F_2 = 2 \text{x} 10^{-9}$ ug/cm^2/sec

The average flux, $\bar{F}_2 = F_2/2 = 10^{-9}$ ug/cm^2-sec.

The resulting concentration can be estimated as:

$$C_t = C_i + (\bar{F}_2 \; A \quad t)/M$$

Where

$C_i = 0$
$\bar{F}_2 = 10^{-9}$ ug/cm^2 s
$A = 314$ cm (for apple of r=5cm)
$t = 360$s
$M = 0.1$kg
$C_t = 10^{-9}$ ug/cm^2 s (314 cm^2) 360s/0.1kg
$= 0.0011$ ug/kg

If partitioning was assumed:

$$S = K \; C_{el}^{\;n}$$

As shown in Equation B-30, the adsorption coefficient may be estimated from the octanol-water partition coefficient.

$K = K_{ow}$ (% lipid)/100
$= 7590$ (0.6)/100
$= 45$

Where apples are assumed to be 0.6% fat.

The Freundlich isotherm parameter (n) is assumed to be 1, unless other information is available, thus

$$S = 45 \ (10 \ ug/L)$$
$$= 450 \ ug/kg$$

It is apparent that in this example, time has not been adequate, and the food piece is too large, for partitioning assumptions to be reasonable.

The uncertainties involved in this analysis are primarily associated with the estimation of an apparent diffusion coefficient and the adsorption coefficient required for equations B-27 and B-28, respectively. Another important point that should be made is that most of the compound that has diffused will be at or near the surface of the apple. Thus, subsequent peeling and trimming could remove these residues almost entirely. The question of time is also important. One hour was chosen as a reasonable estimate of water contact during processing. It would probably be similar for other fruits and vegetables, as few fruits and vegetables are soaked for long periods of time. In any case, a small difference in time would not affect the result greatly. In conclusion, 1 ug/kg could probably be used as an upper limit concentration in fruits and vegetables contaminated from process water containing 10 ug/L benzanthrone.

C.3.3. Absorption from Ambient Water by Fish

A BCF of 523 was estimated using log K_{ow}=3.88. The equation used was:

$$\log BCF = 0.76 \log K_{ow} - 0.23 \text{ (See Table 30)}$$

Using $BCF = 0.048 \ K_{ow}$, a value of 364 is obtained
Using $\log BCF = 1.19 \log K_{oc} - 1.579$
$BCF = 465$

The value for BCF therefore ranges from 360 to 520.

Using Equation B-4, and an estimated BCF of 450:

$$C_{ao} = (BCF) \ C_w / \rho_w$$

where: C_{ao} = concentration of pollutant in aquatic organism at equilibrium (ug/kg)

BCF = bioconcentration factor for fish $\frac{ug/kg}{ug/L}$

C_w = concentration of pollutant in water (ug/L)
ρ_w = density of water (1 kg/L)

thus,

$$C_{ao} = 450 \ (10)/1$$
$$= 4500 \ ug/kg$$